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SOLAR EXTINCTION RADIOMETRY

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I. During this period the work on the spectral line parameters of the OH $\lambda^2\Sigma - X^2\Pi(0,0)$ band has been completed. A detailed paper describing this work has been published in J.Q.S.R.T. and a reprint is enclosed as an Appendix. Numerous reprints requests for this paper were received.

II. Using the methods developed for NO₂ quantification (1) during previous phases of this project, the uv-visible data obtained during the 1977 balloon flights have been used for O₃ quantification.

For atmospheric ozone amounts and the region covered by these spectra, the ozone absorption renders the atmosphere opaque at low sun angles in the 2800-3100Å region (Hartley bands). From about 3500 to 4000Å the ozone absorption coefficients are too small to give appreciable absorption even at the lowest sun angles scanned (~22°). From 4000 to 6000Å (Chappuis bands) the atmospheric absorption is quite weak and broad and does not have the contrast structure required for the three wavelengths method. The region from 3100Å to 3500Å appears to be the best region to use for determining ozone columns with the three-wavelength method.

Accurate determination of ozone columns and volume mixing ratios requires accurate ozone absorption coefficients measured at atmospheric temperatures (210 to 260K). The best presently available published absorption coefficients are those of Vigroux². We have used these coefficients and five combinations of three wavelengths chosen from the features marked in Figure 1

to determine ozone columns and volume mixing ratios.

The ozone volume mixing ratios determined from the 9 February 1977 UV and 17 February 1977 UV data have been compared with standard middle-latitude ozone profiles³. The ozone profiles from both flights are in agreement with the standard profile mixing ratios, as shown in Figure 2.

The spectra in Fig. 1 have been smoothed to 2.5 Å resolution. It should be noted that while the fine structure of the atmospheric O_2 absorption in Fig. 1 is not fully accounted for the Vigroux coefficients, it is in agreement with the recent high resolution (0.2 Å) work being completed at the N.P.S.⁴ The accuracy of the O_2 profiles should improve when this work, which is conducted at atmospheric temperatures, is completed.

III. Work has started on the new UV solar spectra obtained during the 3/19/81 balloon flight. Numerous high and low sun scans were obtained during ascent and from float altitude (~33 km) at 0.02 Å resolution in the 3063-3099 Å region. High and low sun scans from float altitude have been calibrated in wavelength. Representative scans are shown in Fig. 3 and Fig. 4 respectively for the 3070-3082 Å region, which is considered best for OH measurements. The spectra are being studied for OH identification and quantification.

REFERENCES

1. A. Goldman, F.G. Fernald, W.J. Williams and D.G. Murcray, "Vertical Distribution of NO_2 in the Stratosphere as Determined from Balloon Measurements of Solar Spectra in the 4500Å Region," Geophys. Res. Lett. 5, 257 (1978).
2. E. Vigroux, Ann. Phys. 3, 709 (1953); Ann. Phys. 2, 209 (1957); Ann. Phys. 25, 169 (1969).
3. G.L. Mateer, J.J. DeLuise and G.C. Poreo, "The Short-Umkehr Method, Part 1: Standard Ozone Profiles for Use in the Estimation of Ozone Profiles by the Inversion of Short-Umkehr Observations," NOAA Technical Memorandum ERL ARL-56 (1980).
4. A.M. Bass and R.J. Paur, paper WP15, "Absorption Cross-Sections of Ozone as a Function of Temperature," Spectroscopy in Support of Atmospheric Measurements (November 10-12, 1980), Sarasota, Florida.

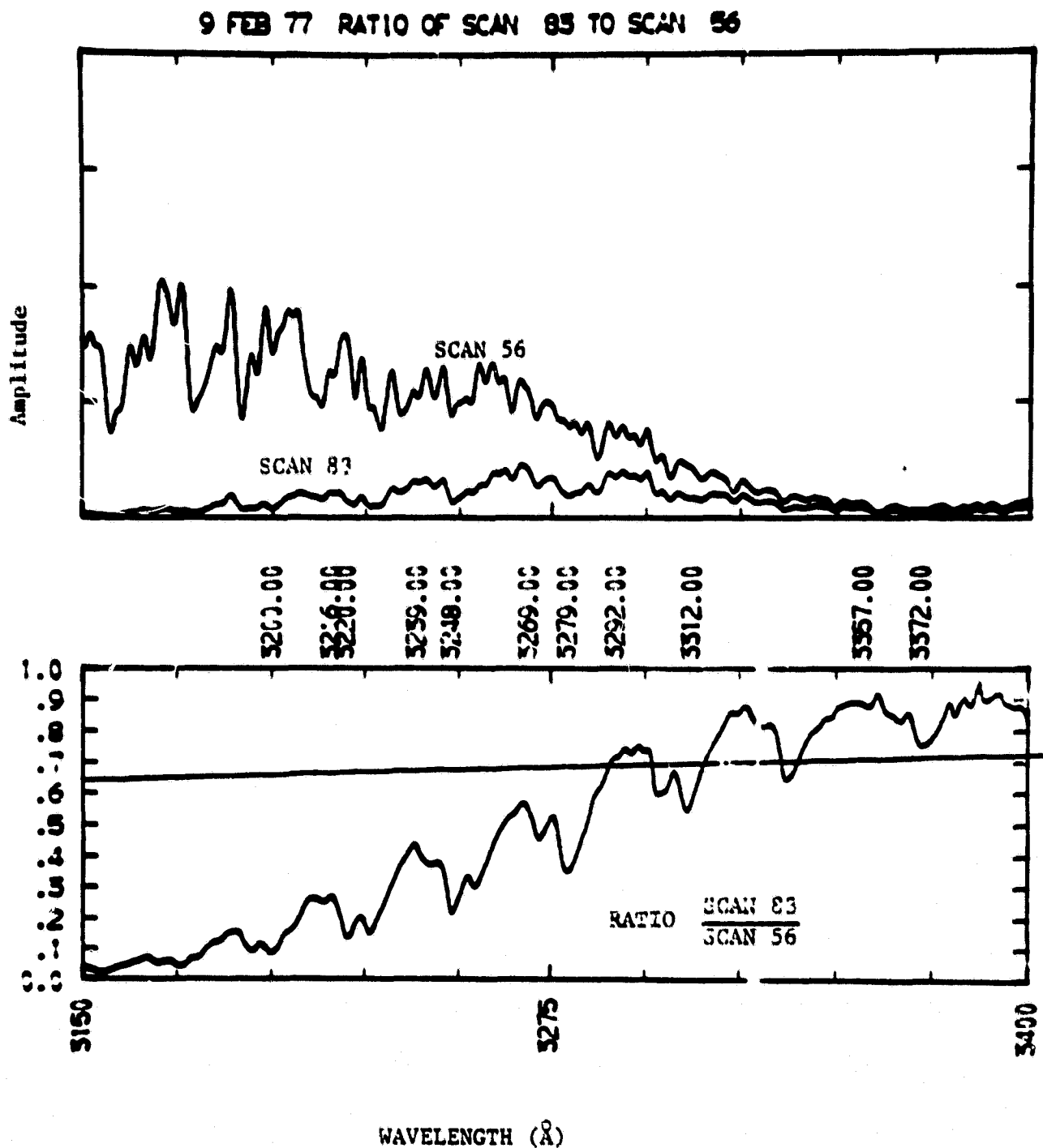


Fig. 1 Ratio of Scan 83 (low sun) to Scan 56 (high sun). The fine structure in the ratio spectrum is due to atmospheric O_3 . Resolution is 2.5\AA .

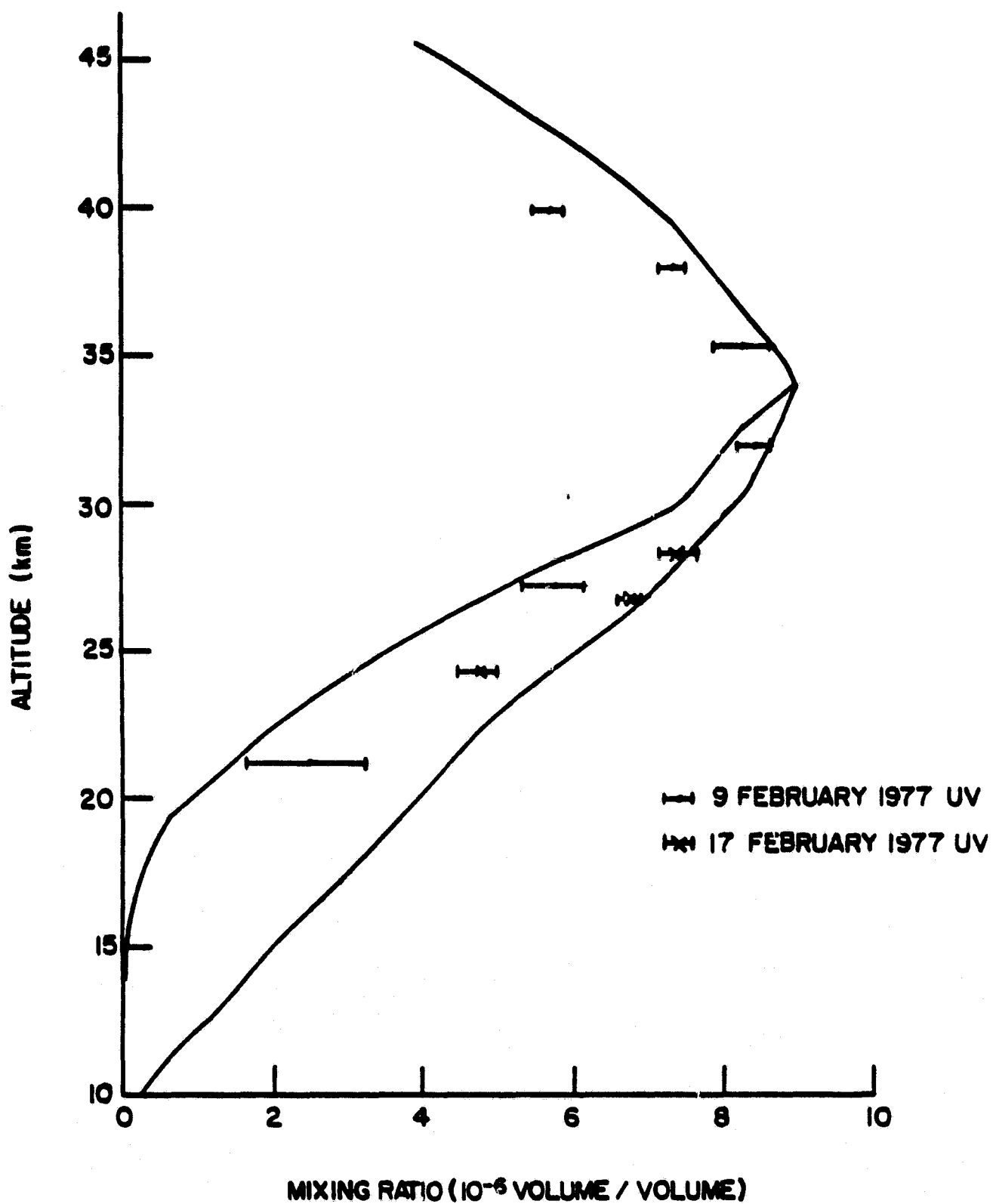


Figure 2 Preliminary ozone profiles superimposed on the standard midlatitude ozone profile of Mateer et al. (1980).

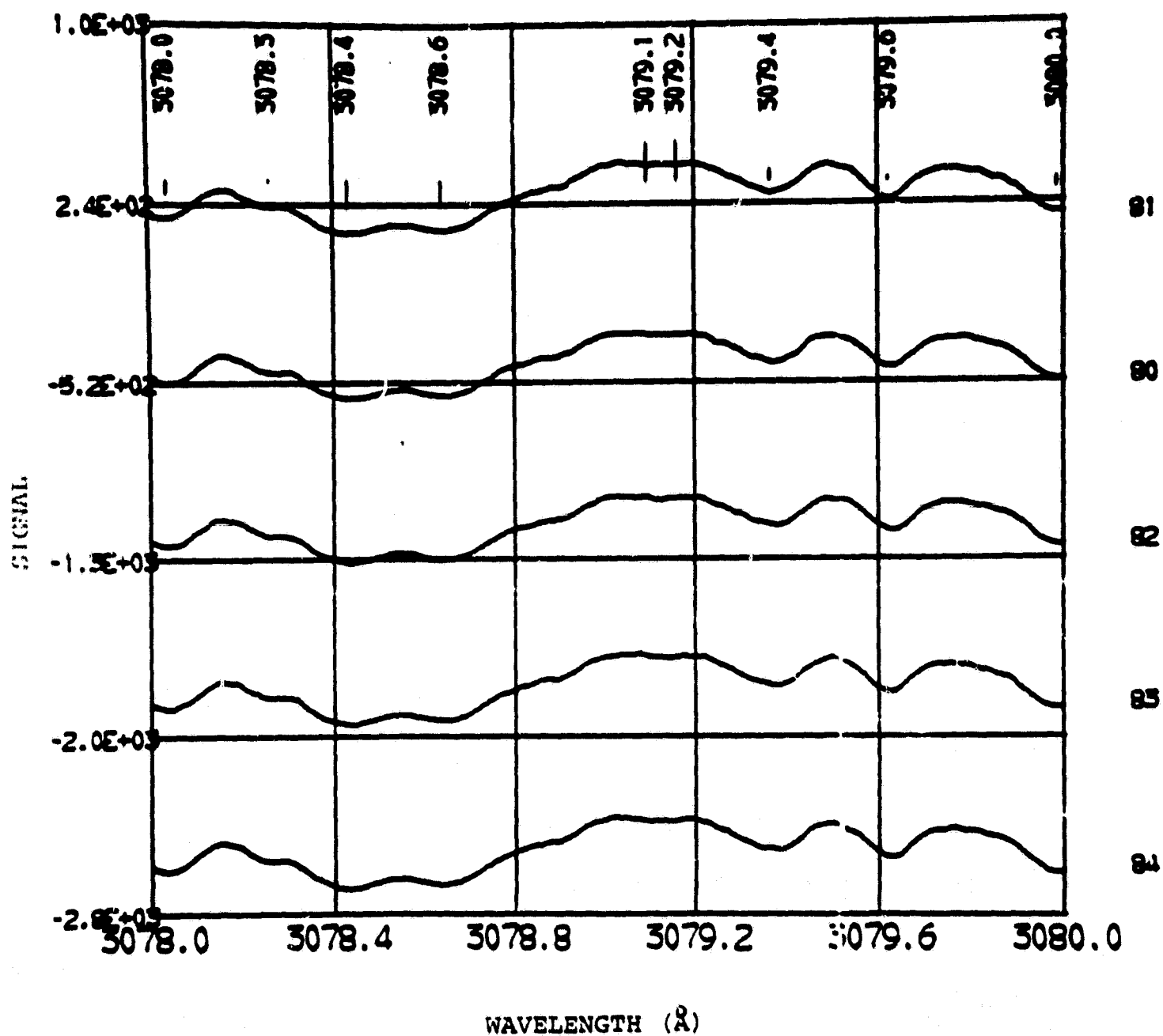


Fig. 3a Selected high sun scans obtained during the 3/19/81 balloon flight from float altitude (33 km). Resolution is 0.03Å.

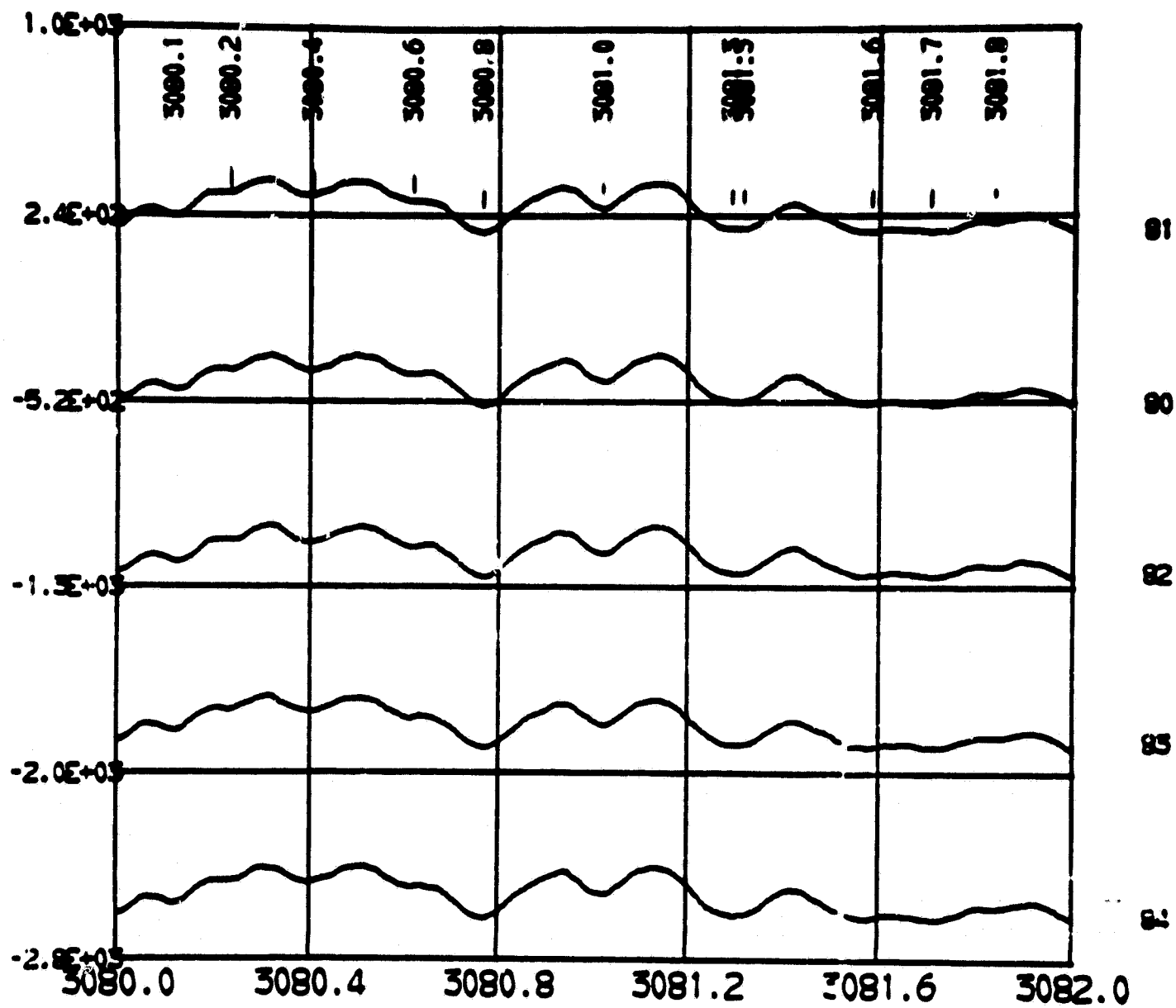


Fig. 3b

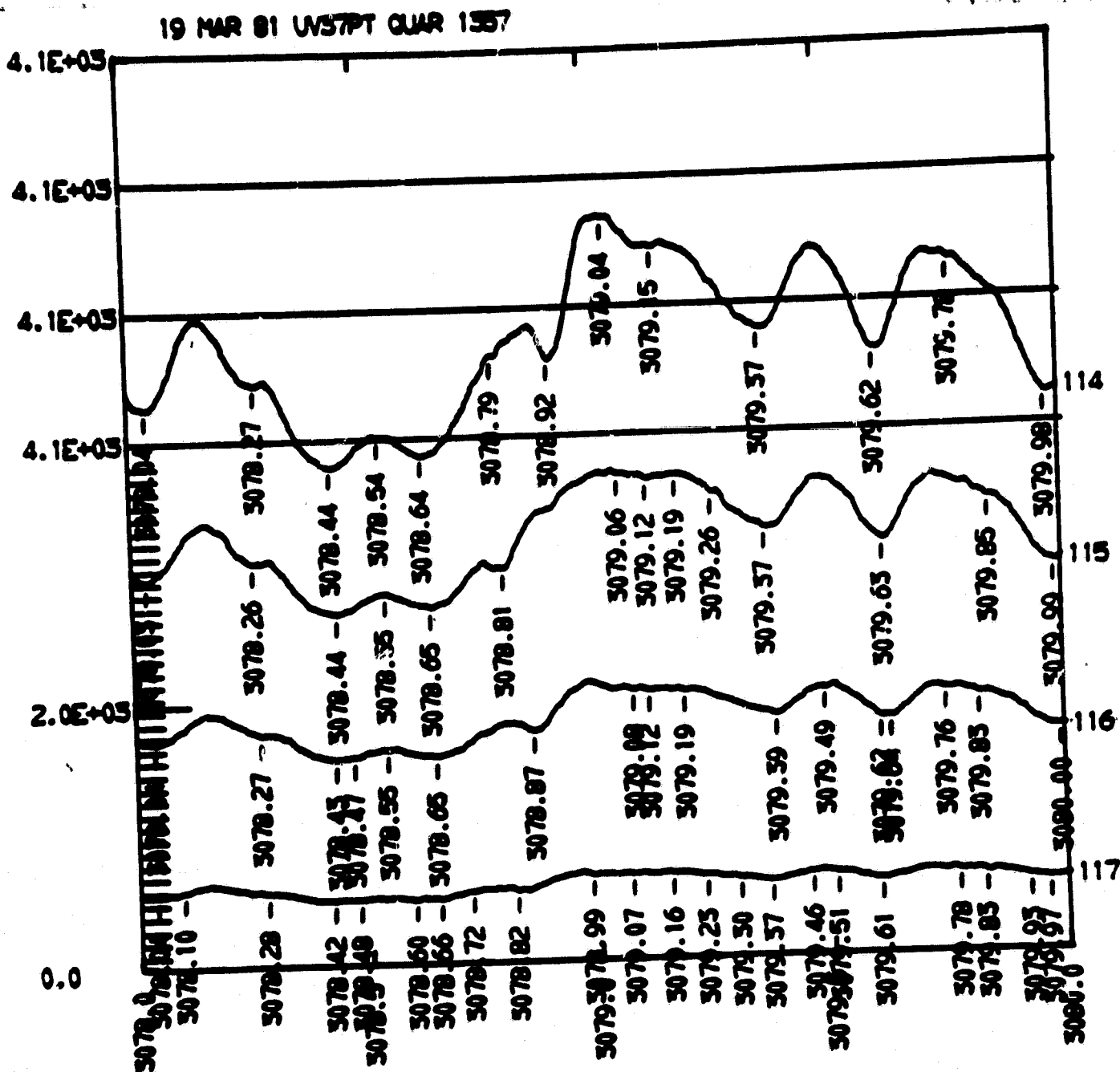


Fig. 4a Selected low sun scans obtained during the 3/19/81 balloon flight from float altitude (33 km). Resolution is 0.03Å.

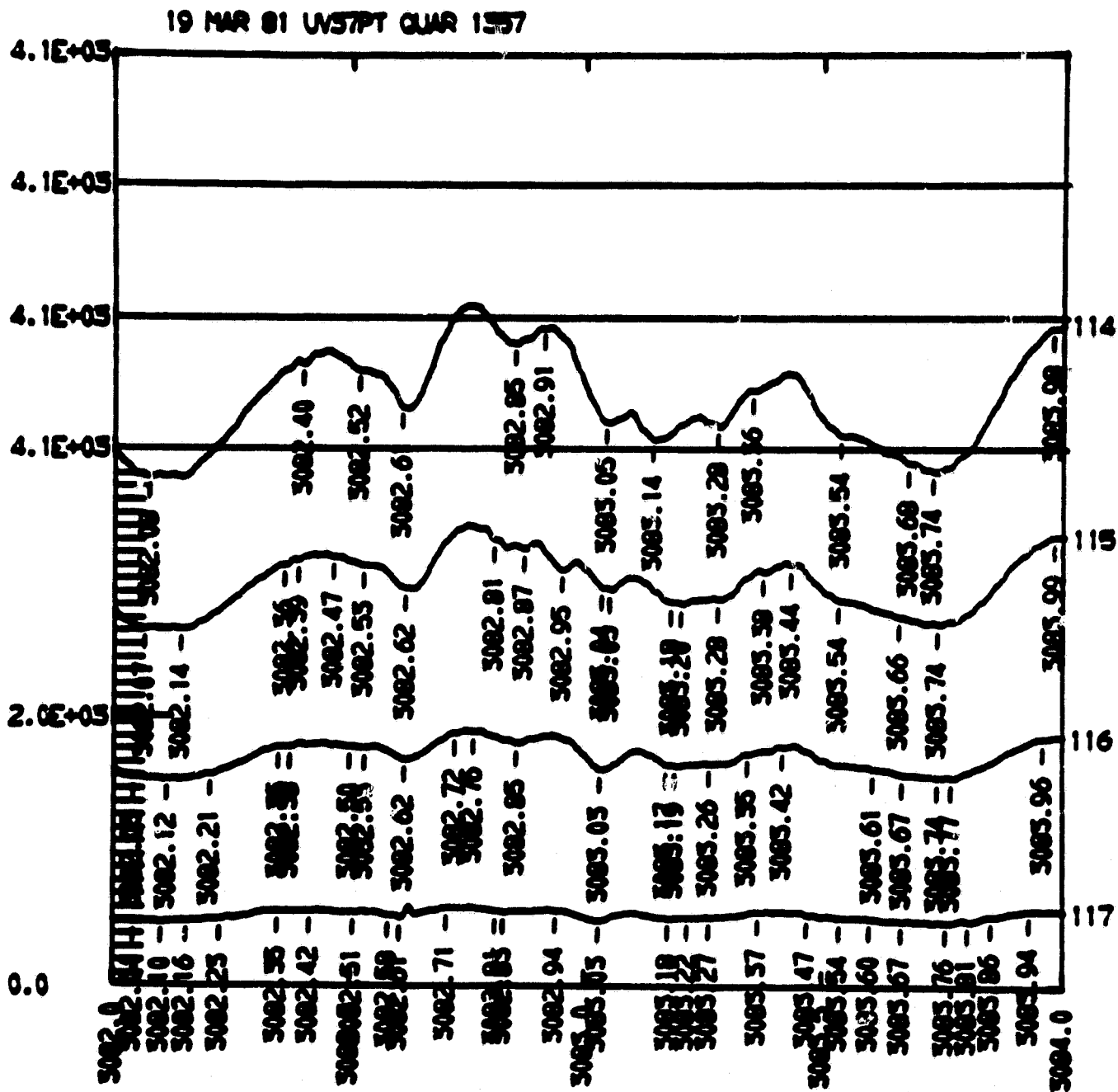


Fig. 4b

SPECTRAL LINE PARAMETERS FOR THE $A^2\Sigma-X^2\Pi(0,0)$ BAND OF OH FOR ATMOSPHERIC AND HIGH TEMPERATURES

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Abstract—Individual spectral line parameters including line positions, strengths, and intensities, have been generated for the $A^2\Sigma-X^2\Pi(0,0)$ band of OH, applicable to atmospheric and high temperatures. Energy levels and transition frequencies are calculated by numerically diagonalizing the Hamiltonian. Line strengths are calculated using the dipole matrix and eigenvectors derived from energy matrix diagonalization. The line strengths are compared to those calculated from previously published algebraic line strength formulas. Tables of line parameters are presented for 240 and 4600°K.

1. INTRODUCTION

The $A^2\Sigma-X^2\Pi(0,0)$ band of OH in the 3085 Å region has been of interest to quantitative spectroscopists for many years because of its high absorption and emission intensity and convenient wavelength location for spectroscopic probes. The hydroxyl radical is a common by-product of most combustion processes, is present in atmospheric, solar and stellar spectra, and in recent years has been also recognized as an important trace constituent in atmospheric chemistry. Accurate determination of the amount of OH present during spectroscopic experiments depends on precise knowledge of line positions and intensities. Several analyses of spectral line positions for this band are available; among the more important of these are those of Dieke and Crosswhite,¹ who provided the first extensive analysis of the OH u.v. spectrum, and Destombes *et al.*,² who performed elaborate analysis of modern microwave, i.r. and u.v. OH data. Intensity (relative and absolute) studies of this band have been reviewed recently by Chidsey and Crosley,³ who also performed extensive RKR calculations of rotational transition probabilities for the A-X system of OH.

The purpose of this work is to combine the best presently available data and theory to derive accurate quantitative line parameters for the $A^2\Sigma-X^2\Pi(0,0)$ band, applicable to atmospheric and high temperatures. The results are displayed in line parameter tables, and include improved values for the line strength, calculated in intermediate coupling from the energy matrix eigenvectors.

2. LINE PARAMETERS DERIVATION

The OH molecule has an unpaired electron with total electronic angular momentum $L = 1$ and $S = 1/2$. In the electronic ground state the projection of L along the internuclear axis is $\Lambda = \pm 1$. The projection of S along the internuclear axis is $\Sigma = \pm 1/2$, with a total electronic angular momentum projection $\Omega = \Lambda + \Sigma$. Here, Λ , Σ , Ω are considered as signed quantities, as in the notation of Hougen.⁴ The electronic ground state is an inverted $^2\Pi$ state with the $^2\Pi_{1/2}(\Omega = \pm 1/2, F_2)$ levels at higher energy than the $^2\Pi_{3/2}$ levels ($\Omega = \pm 3/2, F_1$). The rotational levels for this state are intermediate between Hund's cases (a) and (b). In the $^2\Sigma$ upper state, which is Hund's case (b), $\Lambda = 0$ and $\Omega = \pm 1/2$ with $J = N \pm 1/2$. The $^2\Pi$ and $^2\Sigma$ states perturb one another and produce Λ doubling for each N ($^2\Sigma_{1/2}$) or J ($^2\Pi_{1/2,3/2}$).

We use the unique perturber approximation described by Destombes *et al.*² to calculate energy levels. This process is restricted to a single vibrational level v in the $A^2\Sigma-X^2\Pi$ subspace. The total angular momentum number F (not to be confused with the level designations F_1 and F_2) is a good quantum number. For a given F , the J and $J+1$ levels are weakly coupled by magnetic hyperfine interactions. These interactions are negligible in the calculation of electronic spectra and J may be considered a good quantum number. This procedure gives a 6×6 Hamiltonian matrix, the elements of which are listed in Table 1. The matrix elements are

Table 1. Nonzero Hamiltonian matrix elements (Hund's case (a) basis).

Matrix Elements	Value
$\langle {}^2\Pi_{1/2} H {}^2\Pi_{1/2} \rangle$	$B_n(n^2-2) + \frac{1}{2}D_n(n^2-3) + A_n(n^2-2) + M_n(n^2-3)n^2 + 6$
$\langle {}^2\Pi_{1/2} H {}^2\Pi_{3/2} \rangle$	$B_n n^2 + \frac{1}{2}D_n - D_n(n^2+n^2-1) - A_n n^2 + M_n(n^2+3)n^2 + 2$
$\langle {}^2\Pi_{1/2} H {}^2\Pi_{1/2} \rangle$	$B_n n^2 - 2D_n n^2 + M_n n^2 (3n^2-3n^2+3)$
$\langle {}^2\Pi_{1/2} H {}^2\Sigma_{1/2} \rangle$	$B_n n^2 + \frac{1}{2}D_n + V_0 - D_n(n^2+n^2) + M_n(n^2+3)n^2$
$\langle {}^2\Pi_{1/2} H {}^2\Sigma_{-1/2} \rangle$	$B_n n^2 - 2D_n n^2 + M_n n^2 (3n^2+n^2)$
$\langle {}^2\Pi_{1/2} H {}^2\Sigma_{1/2} \rangle$	$\langle BL_n \rangle \gamma - \langle DL_n \rangle \gamma (2n^2-1) + \langle AL_n \rangle \gamma + \langle ML_n \rangle \gamma (3n^2+1)$
$\langle {}^2\Pi_{1/2} H {}^2\Sigma_{-1/2} \rangle$	$\langle BL_n \rangle \gamma - \langle DL_n \rangle \gamma (2n^2+1) + \langle AL_n \rangle \gamma + \langle ML_n \rangle \gamma (3n^2+6n^2-2)$
$\langle {}^2\Pi_{1/2} H {}^2\Sigma_{1/2} \rangle$	$-2\langle DL_n \rangle \gamma + \langle ML_n \rangle \gamma (2n^2-1) \gamma$
$\langle {}^2\Pi_{1/2} H {}^2\Sigma_{-1/2} \rangle$	$\langle BL_n \rangle \gamma + \frac{1}{2}\langle AL_n \rangle \gamma - \langle DL_n \rangle \gamma (4n^2-1) + \frac{1}{2}\langle AL_n \rangle \gamma (2n^2-1) + \langle ML_n \rangle \gamma (9n^2-3n^2+1)$

Notes:

$$1. \quad m = J \pm 1/2; \quad \gamma = \{(J-1/2)(J+1/2)\}^{1/2}$$

2. Matrix elements are unchanged by exchange of initial and final states or by setting n to $-n$ in both initial and final states.

written in Hund's case (a), with the wave functions represented by $|\Lambda\Sigma\rangle|J\rangle = |\Lambda\Sigma; J\rangle$, so that

$$\begin{aligned} {}^2\Sigma_{+1/2}: \quad |\Lambda\Sigma; J\rangle &= |0^+ 1/2 \pm 1/2; J \pm 1/2\rangle, \\ {}^2\Pi_{+1/2}: \quad |\Lambda\Sigma; J\rangle &= |1 1/2 \pm 1/2; J \pm 1/2\rangle, \\ {}^2\Pi_{+3/2}: \quad |\Lambda\Sigma; J\rangle &= |1 1/2 \pm 1/2; J \pm 3/2\rangle. \end{aligned} \quad (1)$$

The Hamiltonian constants used² are shown in Table 2 (these constants give a better fit to the

Table 2. Hamiltonian constants for $A^2\Sigma-X^2\Pi(0,0)$.

Constant	Value ^a (cm ⁻¹)
B_n	16.9238973
D_n	2.0396602×10^{-3}
M_n	97.7612×10^{-3}
V_0	-7.8199×10^{-3}
A	32402.036239
B_n	-139.228125
B_n	18.3497336
D_n	1.907952×10^{-3}
M_n	0.1239336×10^{-6}
A_n	-0.72330×10^{-3}
$\langle AL_n \rangle$	-131.9226212
$\langle BL_n \rangle$	25.0435400
$\langle DL_n \rangle$	2.6923336×10^{-3}
$\langle AL_n L_n \rangle$	8.051437×10^{-3}
$\langle ML_n \rangle$	0.166603×10^{-6}

^a Values are from Ref. 5 and are rounded to three figures beyond the standard errors indicated in Ref. 2.

observed spectrum than those of Ref. 2, which do not have a sufficient number of digits retained). The 6×6 Hamiltonian matrix may be reduced to two 3×3 blocks by the Kronig transformation.

$$|J\Omega\delta\rangle = \frac{1}{2}(|\Lambda S\Sigma\rangle|J\Omega\rangle + \delta|-\Lambda S-\Sigma\rangle|J-\Omega\rangle), \quad (2)$$

where δ equals s = symmetric = + or a = antisymmetric = -. This notation should not be confused with the s , a and +, - notation for homonuclear diatomic molecules.[†] In this new basis, one of the 3×3 blocks contains only matrix elements of the type $\langle J'\Omega's|H|J\Omega s\rangle$ and the other contains only matrix elements of the type $\langle J'\Omega'a|H|J\Omega a\rangle$.

After numerical diagonalization of a 3×3 Kronig transformed block, the electronic state of each eigenvalue (energy level or, more properly, term value in cm^{-1}) may be determined by noting that the largest eigenvalue belongs to the $^2\Sigma_{1/2}$ state, the intermediate eigenvalue to the $^2\Pi_{1/2}$ state, and the smallest eigenvalue to the $^2\Pi_{3/2}$ state. The remaining quantum numbers and parities may be determined from Table 3.

The selection rules for the $A^2\Sigma-X^2\Pi(0,0)$ electric dipole allowed transitions are $\Delta J = 0, \pm 1$, $\Delta N = 0, \pm 1, \pm 2$. Parity selection rules require $+\leftrightarrow-$, $+\leftrightarrow+$, and $-\leftrightarrow-$, which give for the wavefunction the Kronig symmetry selection rules of $s \leftrightarrow s$ and $a \leftrightarrow a$ for $\Delta J = \pm 1$ (P and R branches) and $s \leftrightarrow a$ for $\Delta J = 0$ (Q branches). Transitions are designated by $^{\Delta N}\Delta J_{F'F}(J'')$ where ' refers to the upper state and '' refers to the lower state and F is F_1 or F_2 . These selection rules permit 12 branches, of which 6 are main branches ($^{\circ}P_{11}$, $^{\circ}Q_{11}$, $^{\circ}R_{11}$, $^{\circ}P_{22}$, $^{\circ}Q_{22}$, $^{\circ}R_{22}$) and 6 are (weaker) satellite branches ($^{\circ}P_{21}$, $^{\circ}Q_{21}$, $^{\circ}R_{21}$, $^{\circ}Q_{12}$, $^{\circ}R_{12}$, $^{\circ}P_{12}$).

The line intensities $S_{lu}(T)$ ($\text{cm}^{-1}/\text{atm-cm}$) at temperature $T(^{\circ}\text{K})$ are calculated from⁶

$$S_{lu}(T) = \frac{1}{8\pi c\nu^2} \left(\frac{N}{p} \right) \frac{e^{-1.4388/T}}{Q_{vR}} A_{ul}^{\circ} (2J'' + 1) (1 - e^{-1.4388/T}), \quad (3)$$

where $\nu (= E' - E'')$ is the transition frequency in cm^{-1} , $c = 2.99792458 \times 10^{10}$ cm/sec , N is the total number of OH molecules/ cm^3 , p is the pressure in atm, A_{ul}° is the Einstein A coefficient in sec^{-1} , E'' is the lower state energy ($= E_l$), and Q_{vR} is the vibration rotation partition function.

Line intensities may be converted from $\text{cm}^{-1}/\text{atm-cm}$ at T to cm/molecule at T by

$$S_{lu}(T)(\text{cm/molecule}) = 3.721963 \times 10^{-20} \frac{T(^{\circ}\text{K})}{273.16(^{\circ}\text{K})} S_{lu}(T)(\text{cm}^{-1}/\text{cm-atm}). \quad (4)$$

The $S_{lu}(T)$ in cm/molecule are at the population temperature.

We assume that Q_{vR} is given by $Q_v Q_R$, where the vibrational partition function Q_v in the harmonic oscillator approximation is

$$Q_v = \frac{1}{1 - e^{-1.4388/\omega_v T}} \quad (5)$$

Table 3. Assignment of quantum numbers to eigenvalues for given J .

State	$^2\Pi_{3/2}$	$^2\Pi_{1/2}$	$^2\Sigma_{1/2}$	
F	1	2	1	2
N	$J-1/2$	$J+1/2$	$J-1/2$	$J+1/2$
Parity: Eigenvalue from				
Symmetric block	$(-1)^{N+1}$	$(-1)^N$	—	$(-1)^N$
Antisymmetric block	$(-1)^N$	$(-1)^{N+1}$	$(-1)^N$	—

[†]We thank J. T. Hougen for pointing out that our notation s = symmetric = + is equivalent to the f levels and a = antisymmetric = - is equivalent to the e levels of J. M. Brown, J. T. Hougen, K.-P. Huber, J. W. C. Johns, I. Kopp, H. Lefebvre-Brion, A. J. Morer, D. A. Ramsay, J. Rostas, and R. N. Zare, *J. Molec. Spectrosc.* **58**, 500 (1975).

and ω_v is the vibrational harmonic oscillator frequency in cm^{-1} . Huber and Herzberg⁷ give $\omega_v = 3737.76 \text{ cm}^{-1}$. A comparison of the values of Q_v calculated by Eq. (5) and by direct summation of $e^{-E_v/T}$ shows a difference of less than 0.2% at 4600°K. The rotational partition function Q_R is calculated from the actual energy levels as follows:

$$Q_R = \sum_{N''} (2J'' + 1) e^{-1.4388 J''(J''+1)/T} \quad (6)$$

Chidsey and Crosley³ give the Einstein A coefficient as

$$A_{v'J',v''J''}^{v'J',v''J''} = \frac{64\pi^4}{3h} p_{v'J',v''J''}^2 S_{J'J''} \nu^3 / (2J' + 1) \text{ sec}^{-1}, \quad (7)$$

where $p_{v'J',v''J''}^2$ is the rovibrational transition probability and $S_{J'J''}$ is the rotational line strength. Chidsey and Crosley tabulate relative values of $A_{v'J',v''J''}^{v'J',v''J''}$ through $N'' = 32$ for the $A^2\Sigma - X^2\Pi(0,0)$ band in their Table 4. They state that they calculated the line strengths $S_{J'J''}$ based on Earls' formulas⁸ with a J -dependent spin-orbit coupling parameter A and the rotational constants of Dieke and Crosswhite.¹ We have found that the use of Earls' formulas can lead to significant errors at high J in the satellite bands. (This problem is further discussed in the following section.) Therefore, we have calculated $S_{J'J''}$ by following the method described by Hougen.⁴ Chidsey and Crosley³ have kindly provided a table of relative values for $p_{v'J',v''J''}^2$ through $J = 35.5$ prior to publication.

The $A_{v'J',v''J''}^{v'J',v''J''}$ may be put on an absolute basis by noting that the lifetime of a state is

$$\tau_{v'J'} = \left(\sum_{v''J''} A_{v'J',v''J''}^{v'J',v''J''} \right)^{-1} \text{ sec.} \quad (8)$$

Because Chidsey and Crosley³ give $A_0^0/A_0^0 \approx 0.0040$ (here the notation is A_v^0), we assume that for the $v' = 0$ vibrational state all vibrational states other than $v'' = 0$ make negligible contributions to $\tau_{v'J'}$. The best available lifetime for the rotationless ($N' = 0$) $v' = 0$ state is probably that measured by German,¹⁰ $\tau_{0,1,2} = (0.688 \pm 0.007) \times 10^{-6} \text{ sec}$. There are three transitions from the $v'' = 0$ state to the rotationless $v' = 0$ state, namely, $^3P_{11}(1.5)$, $^3P_{12}(1.5)$, and $^3Q_{12}(0.5)$. We calculate relative $A_{v'J',v''J''}^{v'J',v''J''}$ for all J' and J'' of interest by ignoring all constant factors in Eq. (7) and normalize these by using Eq. (8).

We form the $S_{J'J''}$ by following the method given by Hougen.⁴ In addition to the selection rules $\Delta J = 0, \pm 1$ and $+\leftrightarrow -$ parity, electric dipole selection rules on Ω give nonzero matrix elements only for $\langle \Omega \pm 1 | \mu_z \pm i\mu_y | \Omega \rangle$ for $\Delta\Omega = \pm 1$ and $\langle \Omega | \mu_z | \Omega \rangle$ for $\Delta\Omega = 0$, where μ_x , μ_y , and μ_z are electric dipole moment components in the molecule fixed axis system. In the laboratory fixed coordinate system

$$\mu_z = \frac{1}{2}(\alpha_{zx} - i\alpha_{zy})(\mu_x + i\mu_y) + \frac{1}{2}(\alpha_{zx} + i\alpha_{zy})(\mu_x - i\mu_y) + \alpha_z\mu_z, \quad (9)$$

where α_{zx} , α_{zy} , and α_z are the direction cosines between the molecule-fixed and laboratory-

Table 4. Nonzero rotational direction cosine matrix elements in $(J'\Omega'|\mu_z|J\Omega)(\text{Hund's case (a)})$.

	$J' = J+1$	$J' = J$	$J' = J-1$
$\langle J, \Omega \mu_z J, \Omega \rangle$	$\left[\frac{(J+\Omega+1)(J-\Omega+1)}{2(J+1)} \right]^{1/2}$	$-\Omega \left[\frac{2J+1}{2J(J+1)} \right]^{1/2}$	$\left[\frac{(J+\Omega)(J-\Omega)}{2J} \right]^{1/2}$
$\langle J, \Omega+1 \mu_z J, \Omega \rangle$	$-\left[\frac{(J+\Omega+1)(J-\Omega+2)}{2(J+1)} \right]^{1/2}$	$\left[\frac{(J-\Omega)(J-\Omega+1)(2J+1)}{2J(J+1)} \right]^{1/2}$	$\left[\frac{(J-\Omega)(J-\Omega-1)}{2J} \right]^{1/2}$
$\langle J, \Omega-1 \mu_z J, \Omega \rangle$	$\left[\frac{(J-\Omega+1)(J-\Omega+2)}{2(J+1)} \right]^{1/2}$	$\left[\frac{(J+\Omega)(J-\Omega+1)(2J+1)}{2J(J+1)} \right]^{1/2}$	$-\left[\frac{(J+\Omega)(J-\Omega-1)}{2J} \right]^{1/2}$

Note: The phases employed here are the same as those used in Refs. 2, 4, and 11.

fixed coordinates systems. The direction cosine matrix elements are given in Table 4. The μ_x , μ_y , and μ_z are taken to be experimentally determined parameters. For lack of better information, we take $\sqrt{(1/2)}|\mu_x + i\mu_y| = \sqrt{(1/2)}|\mu_x - i\mu_y| = \mu_z = 1$.

Because we assume that the electronic and rotational parts of the wavefunction are separable, the electric dipole matrix elements may be written as

$$\begin{aligned} \langle \Lambda'S'\Sigma'; J'\Omega' | \mu_z | \Lambda S \Sigma; J \Omega \rangle &= \frac{1}{2} \langle \Lambda'S'\Sigma' | \mu_x + i\mu_y | \Lambda S \Sigma \rangle \langle J'\Omega' | a_{zx} - ia_{zy} | J \Omega \rangle \\ &+ \frac{1}{2} \langle \Lambda'S'\Sigma' | \mu_x - i\mu_y | \Lambda S \Sigma \rangle \langle J'\Omega' | a_{zx} + ia_{zy} | J \Omega \rangle + \langle \Lambda'S'\Sigma' | \mu_z | \Lambda S \Sigma \rangle \langle J'\Omega' | a_{zz} | J \Omega \rangle, \end{aligned} \quad (10)$$

where " has been dropped on the lower state quantities. Only one of the three terms on the r.h.s. of Eq. (10) is nonzero for any allowed transition matrix element. The electric dipole transition matrix is formed in the same basis as was the Hamiltonian matrix, that is, the Hund's case (a) basis. Selection rules in this basis are $\Delta S = 0$, $\Delta \Sigma = 0$, $\Delta \Lambda = 0, \pm 1$, and $\Delta J = 0, \pm 1$. Because $\Delta \Sigma = 0$ and $\Omega = \Lambda + \Sigma$, the selection rule $\Delta \Omega = \Delta \Lambda$ is obtained.

For $^2\Sigma-^2\Pi$ transitions the last term in Eq. (10) is always zero. Because we are interested in $^2\Sigma-^2\Pi$ transitions, we set all matrix elements of the type $\langle ^2\Sigma | \mu_z | ^2\Sigma \rangle$ and $\langle ^2\Pi | \mu_z | ^2\Pi \rangle$ equal to zero. This approximation is valid because these matrix elements are much smaller in magnitude than the $\langle ^2\Sigma | \mu_z | ^2\Pi \rangle$ matrix elements and because they enter into the line strength only through weak mixing between the $^2\Pi$ and $^2\Sigma$ wavefunctions. The relative phases of the matrix elements are determined by following the prescription of Hougen⁴ and Whiting and Nicholls.¹¹ Following the suggestions of Whiting and Nicholls, we have normalized the line strengths so that

$$\sum_{J', J''} S_{J', J''} = 2(2S+1)(2J''+1) = 4(2J''+1). \quad (11)$$

Table 4 reflects this choice of normalization.

The line strength $S_{J', J''}$ is formed in intermediate coupling by taking $|\langle \mu | \mu_z | I \rangle|^2$, where $|\mu\rangle$ represents the eigenvector of the $^2\Sigma$ state, $|I\rangle$ represents the eigenvector of the $^2\Pi$ state, and μ_z now represents the 6×6 transition matrix. However, the eigenvectors formed during diagonalization of the energy matrices are in the Kronig transformed basis; therefore, the dipole matrix must also be transformed into this basis. Using the Kronig transformed wavefunctions given by Eq. (1), the Kronig transformed dipole matrix elements have the form

$$\begin{aligned} \langle J'\Omega'\delta' | \mu_z | J\Omega\delta \rangle &= \frac{1}{2} (\langle J'\Omega' | \mu_z | J\Omega \rangle + \delta \langle J'\Omega' | \mu_z | J-\Omega \rangle) \\ &+ \delta' \langle J'-\Omega' | \mu_z | J\Omega \rangle + \delta\delta' \langle J'-\Omega' | \mu_z | J-\Omega \rangle \end{aligned} \quad (12)$$

and, if we let μ_z^δ be the matrix of the $\langle J'\Omega'\delta' | \mu_z | J\Omega\delta \rangle$,

$$S_{J', J''} = |\langle J'\Omega'\delta' | \mu_z^\delta | J\Omega\delta \rangle|^2. \quad (13)$$

To our knowledge, the $^2\Sigma-^2\Pi$ transition matrices have not been published elsewhere. We show them for the P, Q, and R branches in Tables 5-7. The twelve branches correspond to the four 3×3 blocks in the Kronig basis as follows:

$$\left(\begin{array}{c|c} \begin{array}{c} a \leftarrow a \\ {}^P P_{11}, {}^R R_{11}, {}^O P_{12}, {}^O R_{12} \end{array} & \begin{array}{c} a \leftarrow s \\ {}^O Q_{11}, {}^P Q_{12} \end{array} \\ \hline \begin{array}{c} s \leftarrow a \\ {}^O Q_{22}, {}^R Q_{21} \end{array} & \begin{array}{c} s \leftarrow s \\ {}^P P_{22}, {}^R R_{22}, {}^O P_{21}, {}^S R_{21} \end{array} \end{array} \right) \quad (14)$$

For the Q-branch lines, the only nonzero 3×3 blocks are those for $a \leftarrow s$ and $s \leftarrow a$, while, for the R- and P-branch lines, the only nonzero 3×3 blocks are those for $a \leftarrow a$ and $s \leftarrow s$. When forming line strengths, the appropriate block must be substituted into Eq. (13) for μ_z^δ . For

Table 5. P-branch $^2\Sigma^+ - ^2\Pi$ transition matrix.

i) Hund's case (a) basis				ii) Kronig basis									
$2\Pi_{-3/2}$	$2\Pi_{-1/2}$	$2\Sigma_{-1/2}$	$2\Pi_{1/2}$	$2\Pi_{-3/2}$	$2\Pi_{-1/2}$	$2\Sigma_{-1/2}$	$2\Pi_{1/2}$	$2\Pi_{3/2}$	$2\Sigma_{1/2}$	$2\Pi_{1/2}$	$2\Pi_{3/2}$	$2\Sigma_{3/2}$	$2\Pi_{3/2}$
0	0	-w	0	0	0	0	0	0	-w	0	0	0	0
0	0	0	-x	0	0	0	0	0	x	0	0	0	0
-w	0	0	0	0	-x	0	0	-w	0	0	0	0	0
0	-x	0	0	0	0	0	-w	0	0	0	0	0	0
0	0	-x	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	-w	0	0	0	0	0	0	0	0	0

$$w = \left[\frac{15^3/2}{2J} \right]^{1/2} v_A$$

$$x = \left[\frac{1^3/2}{2J} \right]^{1/2} v_A$$

$$\text{where } v_A = \sqrt{3} |u_x u_y| = 1$$

Table 6. Q-branch $^2\Sigma - ^2\Pi$ transition matrix.

1) Hund's case (a) basis				2) Kronig basis									
$2H_{-3/2}$	$2H_{-1/2}$	$2H_{1/2}$	$2H_{3/2}$	$2H_{-3/2}$	$2H_{-1/2}$	$2H_{1/2}$	$2H_{3/2}$	$2H_{-3/2}$	$2H_{-1/2}$	$2H_{1/2}$	$2H_{3/2}$	$2H_{-3/2}$	$2H_{-1/2}$
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
-t	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-v	0	0	0	0	0	0	0	0	0	0	0	0
0	0	v	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

$$t = \frac{(1-1/2)(1+3/2)(2J+1)}{2J(J+1)} \frac{1}{2} v_A$$

$$v = \frac{(1+1/2)(2J+1)}{2J(J+1)} \frac{1}{2} v_A$$

where $v_A = \sqrt{6} |v_{\Sigma} - v_{\Pi}| = 1$

Table 7. R-branch ${}^3\Sigma^- \rightarrow {}^1\Pi$ transition matrix.

1) Hund's case (a) basis	2) Kronig basis											
	${}^3\Pi_{-3/2}$	${}^3\Pi_{-1/2}$	${}^3\Sigma_{-1/2}$	${}^3\Pi_{1/2}$	${}^3\Pi_{3/2}$	${}^3\Sigma_{1/2}$	${}^3\Pi_{-3/2}$	${}^3\Pi_{-1/2}$	${}^3\Sigma_{-1/2}$	${}^3\Pi_{1/2}$	${}^3\Pi_{3/2}$	${}^3\Sigma_{1/2}$
${}^3\Pi_{-3/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Pi_{-1/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Sigma_{-1/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Pi_{1/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Pi_{3/2}$	0	0	0	0	0	0	0	0	0	0	0	0

${}^3\Pi_{-3/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Pi_{-1/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Sigma_{-1/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Pi_{1/2}$	0	0	0	0	0	0	0	0	0	0	0	0
${}^3\Pi_{3/2}$	0	0	0	0	0	0	0	0	0	0	0	0

$$y = \frac{(3-1/2)(3+1/2)}{2(3+1)} \frac{1}{2} v_A$$

$$z = \frac{(3+1/2)(3-1/2)}{2(3+1)} \frac{1}{2} v_A$$

where $v_A = \sqrt{1/2} [v_x^2 + v_y^2] = 1$

example, to generate the Q_1 line strength we form

$$S^Q_{J_1, J_2} = |\langle \psi_{J_1, J_2}^t | (a \leftarrow s) | \psi_{J_1, J_2}^t \rangle|^2. \quad (15)$$

3. RESULTS AND DISCUSSION

Line strengths, Einstein A coefficients, intensities, and transition frequencies have been calculated for all branches of the $A^2\Sigma-X^2\Pi(0,0)$ OH spectrum through $J = 15.5$ at 240°K for atmospheric applications and through $J = 40.5$ at 4600°K for high temperature applications. These calculated values are shown in Tables 8 and 9, respectively. The total band intensities (by summation of the individual lines) are $2.7948 \times 10^4 \text{ cm}^{-1}/\text{atm-cm}$ at 240°K and $8.6863 \times 10^2 \text{ cm}^{-1}/\text{atm-cm}$ at 4600°K. Line intensities are plotted at these two temperatures in Fig. 1. Some caution must be exercised in using high J data from Table 9. The spectroscopic constants¹ used here were determined from data² which included transitions through $J = 25.5$. Although these constants allow prediction of that data to within 0.1 cm^{-1} maximum error and a standard deviation of $\sim 0.03 \text{ cm}^{-1}$ (the hyperfine structure is neglected here), such accuracy cannot be expected for all lines between $J = 25.5$ and 40.5. Uncertainties in the calculation of energy levels at these high J cause proportionally smaller uncertainties in the energy eigenvectors (wavefunctions) and in quantities calculated using the eigenvectors (line strengths, Einstein A coefficients, and intensities).

Chidsey and Crosley⁹ list $p_{J_1, J_2}^{P, Q, R}$ through $J = 35.5$. We have extrapolated $p_{J_1, J_2}^{P, Q, R}$ for $J = 36.5$ –40.5. Although the dependence of $p_{J_1, J_2}^{P, Q, R}$ on J is quite linear for P, Q, and R transition probabilities between $J = 25.5$ and 35.5, extrapolated $p_{J_1, J_2}^{P, Q, R}$ used to calculate Einstein A coefficients and intensities at higher J must be used with caution.

Although we list four digits for Einstein A coefficients and intensities in Tables 8 and 9, the absolute uncertainties of these quantities cannot be less than 1%, because German's¹⁰ $\tau_{0,1/2}$ has a 1% quoted uncertainty and because Chidsey and Crosley's⁹ $p_{J_1, J_2}^{P, Q, R}$ are quoted to three significant digits. The relative uncertainties are limited by the relative accuracy of the $p_{J_1, J_2}^{P, Q, R}$ and the line strengths. These relative uncertainties should be less than 0.5% for J less than 25.5 and are probably less than 1% for J less than 35.5.

Our calculated line strengths have been checked for accuracy by comparison with values calculated using Earls¹¹ algebraic formulas (these formulas are equivalent to those of Kovacs¹² for $^2\Sigma-^2\Pi$ transitions). When centrifugal and higher order distortion and $\Sigma-\Pi$ interactions are

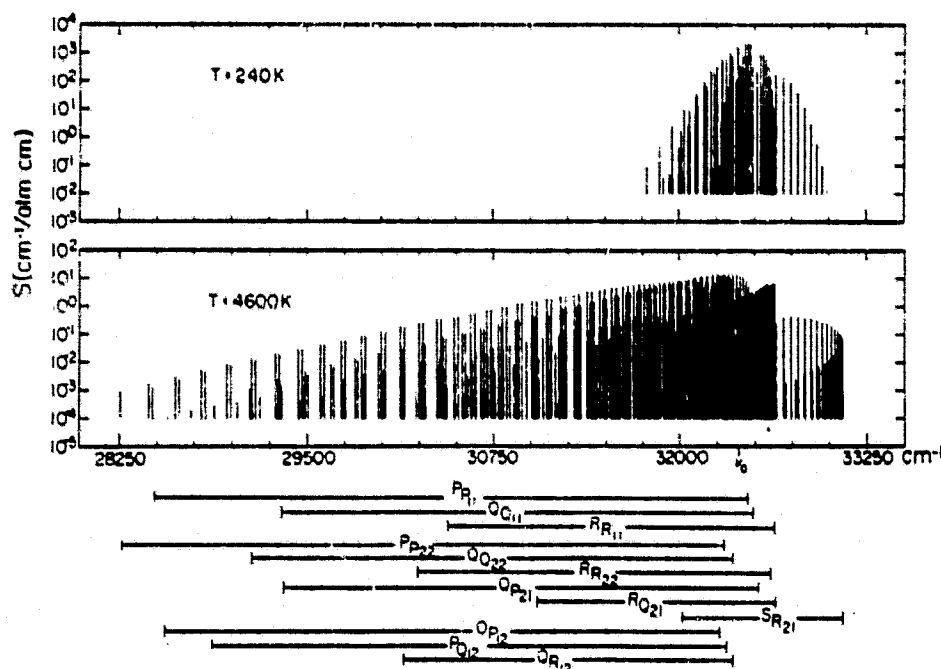


Fig. 1. Line intensities and positions for the $A^2\Sigma-X^2\Pi(0,0)$ band of OH. Only lines with intensity greater than 10^{-5} the intensity of the strongest line have been plotted.

Table 8. Line parameters for the $A^1\Sigma^+-X^1\Pi(0,0)$ OH band at 240°K.

J'	J''	Lower energy vacuum cm ⁻¹	Transition	Frequency vacuum cm ⁻¹	Wavelength SIP angstroms	Intensity cm ⁻² atm ⁻¹	Intensity cm/molecule	Einstein sec ⁻¹	Line strength	Number
T = 240 K										
14.5	15.5	4939.922	0 P 1 2(15,5)	30975.003	3227.4696	2.110E-11	6.325E-34	3.910E+03	2.20301E-01	1
13.5	14.5	4377.419	0 P 1 2(14,5)	31004.603	3216.0096	6.649E-10	2.174E-29	4.547E+03	2.31000E-01	2
12.5	13.5	3846.059	0 P 1 2(13,5)	31191.092	3205.0352	1.729E-09	5.659E-28	5.329E+03	2.32030E-01	3
11.5	12.5	3348.000	0 P 1 2(12,5)	31296.666	3194.1051	3.704E-07	1.213E-26	6.200E+03	2.36976E-01	4
10.5	11.5	2804.110	0 P 1 2(11,5)	31390.949	3183.0992	6.515E-06	2.133E-25	7.400E+03	2.72606E-01	5
14.5	15.5	4932.933	0 P 2 2(15,5)	31460.396	3177.6003	1.623E-09	5.307E-29	2.965E+05	1.59630E-01	6
15.5	15.5	4932.933	0 P 0 1 2(15,5)	31463.010	3177.3155	7.679E-11	2.444E-30	1.200E+04	7.57344E-01	7
9.5	10.5	2453.149	0 P 1 2(10,5)	31490.667	3173.0193	9.373E-05	3.064E-24	9.003E+03	2.90335E-01	8
13.5	14.5	4371.365	0 P 2 2(14,5)	31540.460	3169.6197	4.517E-08	1.477E-27	3.047E+05	1.49196E-01	9
14.5	14.5	4371.365	0 P 0 1 2(14,5)	31543.620	3169.2961	2.333E-09	7.420E-29	1.470E+04	7.91544E-01	10
14.5	15.5	4341.046	0 P 1 1(15,5)	31573.139	3166.3329	5.750E-08	1.800E-27	3.059E+05	1.62750E-01	11
8.5	9.5	2056.568	0 P 1 2(9,5)	31595.731	3164.0607	1.099E-03	3.595E-23	1.094E+04	1.10306E-01	12
12.5	13.5	3841.676	0 P 2 2(13,5)	31617.404	3161.2990	1.033E-06	3.170E-26	3.170E+05	1.10917E-01	13
13.5	13.5	3841.676	0 P 0 1 2(13,5)	31623.425	3161.5977	6.019E-08	1.960E-27	1.710E+04	0.10293E-01	14
13.5	14.5	3694.759	0 P 1 1(14,5)	31651.363	3158.5092	1.337E-06	4.371E-26	3.172E+05	1.52695E-01	15
7.5	8.5	1694.914	0 P 1 2(8,5)	31595.020	3154.6534	1.040E-12	3.420E-32	1.352E+04	3.32902E-01	16
11.5	12.5	3344.522	0 P 2 2(12,5)	31691.411	3150.5157	1.926E-05	6.299E-25	3.267E+05	1.28593E-01	17
12.5	12.5	3344.522	0 P 0 1 2(12,5)	31694.220	3150.2351	1.200E-06	4.107E-26	2.005E+04	0.74207E-01	18
12.5	13.5	3311.902	0 P 1 1(13,5)	31726.769	3151.8001	2.547E-05	8.330E-25	3.209E+05	1.42615E-01	19
10.5	11.5	2800.525	0 P 2 2(11,5)	31762.432	3167.4639	2.920E-04	9.549E-24	3.363E+05	1.10217E-01	20
11.5	11.5	2800.525	0 P 0 1 2(11,5)	31765.021	3167.2054	2.235E-05	7.310E-25	2.359E+04	9.24997E-01	21
6.5	7.5	1360.720	0 P 1 2(7,5)	31701.413	3145.5021	0.077E-02	2.641E-21	1.695E+04	3.57791E-01	22
11.5	12.5	2846.009	0 P 1 1(12,5)	31799.454	3143.7972	3.954E-04	1.293E-23	1.695E+05	1.32510E-01	23
9.5	10.5	2450.279	0 P 2 2(10,5)	31830.303	3140.7625	3.575E-03	1.170E-22	3.449E+05	1.07700E-01	24
10.5	10.5	2450.279	0 P 0 1 2(10,5)	31832.700	3140.5061	3.195E-04	1.045E-23	2.001E+04	0.80044E-01	25
10.5	11.5	2413.613	0 P 1 1(11,5)	31869.446	3136.0927	4.904E-03	1.530E-22	3.510E+05	1.22402E-01	26
5.5	6.5	1070.509	0 P 1 2(6,5)	31869.705	3136.0672	5.003E-01	1.530E-20	2.162E+04	3.04410E-01	27
8.5	9.5	2054.353	0 P 2 2(9,5)	31895.203	3136.3516	3.925E-02	1.353E-21	3.532E+05	9.72727E-00	28
9.5	9.5	2054.353	0 P 0 1 2(9,5)	31897.463	3136.1373	3.724E-03	1.210E-22	3.359E+04	1.04530E-00	29
9.5	10.5	2015.036	0 P 1 1(10,5)	31936.701	3130.2707	5.079E-02	1.661E-21	3.629E+05	1.12265E-01	30
4.5	5.5	824.013	0 P 1 2(5,5)	31954.665	3120.5267	2.476E-08	8.092E-28	2.019E+04	4.10930E-01	31
7.5	8.5	1693.290	0 P 2 2(8,5)	31957.040	3120.2934	2.779E-01	9.009E-21	3.611E+05	6.66026E-00	32
8.5	8.5	1693.290	0 P 0 1 2(8,5)	31959.000	3120.1015	3.530E-02	1.154E-21	4.077E+04	1.11850E-00	33
15.5	15.5	4939.902	0 P 2 2(15,5)	31963.173	3127.6939	3.010E-09	9.442E-29	5.549E+05	3.12030E-01	34
8.5	9.5	1650.790	0 P 1 1(9,5)	32001.569	3123.9470	4.172E-01	1.364E-20	3.745E+05	1.02106E-01	35
6.5	7.5	1367.617	0 P 2 2(7,5)	32015.507	3122.5733	1.740E-08	5.609E-28	3.600E+05	7.59004E-00	36
14.5	14.5	4377.619	0 P 0 2 2(14,5)	32015.910	3122.5417	0.436E-08	2.975E-27	5.712E+05	2.92491E-01	37
7.5	7.5	1367.617	0 P 0 1 2(7,5)	32017.324	3122.4330	2.712E-01	9.076E-21	5.020E+04	1.20092E-00	38
15.5	14.5	4377.619	0 P 1 2(14,5)	32019.325	3122.2007	1.434E-09	4.690E-25	9.105E+03	5.12512E-01	39
3.5	4.5	600.194	0 P 1 2(4,5)	32035.976	3120.5450	9.645E-08	3.154E-19	3.767E+04	4.32924E-01	40
14.5	15.5	4351.310	0 P 2 2(14,5)	32042.018	3119.9973	1.000E-09	6.175E-29	1.095E+04	5.57413E-01	41
15.5	15.5	4351.310	0 P 0 1 1(15,5)	32045.433	3119.6649	1.026E-07	3.354E-27	5.577E+05	3.12018E-01	42
7.5	8.5	1321.252	0 P 1 1(8,5)	32063.690	3117.0005	2.751E-08	8.997E-28	3.060E+05	9.19253E-00	43
13.5	13.5	3846.059	0 P 2 2(13,5)	32064.906	3117.7702	1.939E-06	6.341E-26	5.066E+05	2.72106E-01	44
14.5	13.5	3846.059	0 P 1 2(14,5)	32060.126	3117.4571	3.742E-08	1.224E-27	1.050E+04	5.40150E-01	45
5.5	6.5	1077.054	0 P 2 2(6,5)	32070.760	3117.2004	0.575E-08	2.004E-19	3.737E+05	6.52103E-00	46
6.5	6.5	1077.054	0 P 0 1 2(6,5)	32072.279	3117.0534	1.600E-08	5.493E-20	6.270E+04	1.29194E-00	47

13.5	14.5	3019.156	-	0	2	1 1 1 4 .51	32092.600	3115.0709	4.930E-00	1.615E-27	1.247E+04	5.05109E-01	68
14.5	14.5	3019.156	-	0	0	1 1 1 4 .51	32095.029	3115.7663	2.396E-06	7.035E-26	5.735E+05	2.91665E+01	69
12.5	12.5	3168.000	0	0	2	2 1 2 .51	32110.200	3113.3722	3.630E-05	1.190E-24	6.022E+05	2.91665E+01	50
2.5	2.5	429.275	-	0	0	1 2 1 3 .51	32113.223	3113.3001	2.091E+01	9.453E-19	5.179E+04	4.40594E-01	51
13.5	12.5	3368.000	0	0	0	1 2 1 2 .51	32113.222	3113.0792	0.042E-07	2.630E-26	1.232E+04	5.71274E-01	52
4.5	5.5	426.525	0	0	2	2 1 5 .51	32122.605	3112.1932	3.293E+01	1.077E-13	3.785E+05	5.63172E+00	53
6.5	7.5	1026.730	-	0	0	1 1 1 7 .51	32123.403	3112.0925	1.669E+01	6.730E-19	3.907E+05	6.17260E+00	54
5.5	5.5	824.525	0	0	0	1 2 1 5 .51	32123.609	3112.0644	0.346E+00	2.724E-19	7.991E+04	1.30074E+00	55
12.5	13.5	3319.355	0	0	0	2 1 1 3 .51	32139.725	3110.6065	1.060E-05	3.499E-26	1.479E+04	6.16716E-01	56
13.5	12.5	3319.355	0	0	0	1 1 1 3 .51	32142.747	3110.2196	4.570E-05	1.497E-24	5.000E+05	2.71260E+01	47
11.5	11.5	2004.110	-	0	0	2 2 1 1 .51	32151.022	3109.3416	5.539E-04	1.011E-23	6.120E+05	2.31170E+01	58
12.5	11.5	2004.110	-	0	0	1 2 1 1 .51	32154.640	3109.0691	1.441E-04	4.041E-25	1.447E+04	6.06610E-01	59
3.5	4.5	600.100	-	0	0	2 2 1 4 .51	32170.237	3107.5617	9.696E+01	3.171E-10	3.019E+05	4.33399E+00	60
4.5	4.5	600.104	-	0	0	1 2 1 4 .51	32171.240	3107.4600	3.292E+01	1.077E-10	1.037E+05	1.44363E+00	61
5.5	6.5	767.450	0	0	0	1 1 1 6 .51	32180.756	3106.5659	6.067E+01	1.904E-10	4.161E+05	7.19204E+00	62
11.5	12.5	2052.605	-	0	0	2 1 1 2 .51	32183.440	3106.2060	1.095E-05	6.202E-25	1.737E+04	6.32643E-01	63
1.5	2.5	200.769	0	0	0	1 2 1 2 .51	32185.009	3106.6542	6.333E+01	2.071E-10	7.357E+04	6.13554E-01	64
12.5	12.5	2052.605	-	0	0	1 1 1 2 .51	32186.266	3106.0161	7.126E-04	2.330E-23	6.025E+05	2.50914E+01	65
16.5	10.5	2633.169	0	0	0	2 2 1 0 .51	32189.707	3105.6743	5.019E-03	2.230E-22	5.220E+05	2.10604E+01	66
11.5	10.5	2633.169	0	0	0	1 2 1 0 .51	32192.397	3105.4225	2.046E-04	6.952E-24	1.711E+04	6.46105E-01	67
2.5	3.5	429.450	0	0	0	2 2 1 3 .51	32213.092	3103.3503	2.127E+02	6.954E-10	3.035E+05	3.23470E+00	68
3.5	3.5	429.454	0	0	0	1 2 1 3 .51	32214.713	3103.2712	1.014E+02	3.370E-10	1.377E+05	1.55030E+00	69
10.5	11.5	2619.001	0	0	0	2 1 1 1 .51	32224.095	3102.3960	2.766E-04	9.403E-24	2.066E+04	6.91759E-01	70
9.5	9.5	2056.560	-	0	0	2 2 1 9 .51	32226.466	3102.1396	5.746E-02	2.204E-21	6.293E+05	1.07962E+01	71
11.5	11.5	2619.001	0	0	0	1 1 1 1 .51	32226.466	3102.1396	0.908E-03	2.939E-22	6.139E+05	2.30299E+01	72
10.5	9.5	543.575	-	0	0	1 1 1 1 .51	32226.492	3102.1364	2.611E+02	6.376E-10	4.319E+05	6.13324E+00	73
4.5	5.5	209.041	-	0	0	2 2 1 2 .51	32252.008	3099.6007	3.293E+02	1.077E-17	3.040E+05	2.14901E+00	74
1.5	1.5	107.491	-	0	0	1 2 1 1 .51	32253.049	3099.5025	0.761E+01	2.065E-10	1.114E+05	3.10162E-01	75
2.5	2.5	209.341	-	0	0	1 2 1 2 .51	32253.647	3099.5463	4.607E+02	7.070E-10	1.075E+05	1.57735E+00	76
0.5	0.5	1694.914	0	0	0	2 2 1 0 .51	32256.722	3099.4217	5.330E-01	1.744E-20	6.343E+05	1.59234E+01	77
9.5	0.5	1694.914	0	0	0	1 2 1 0 .51	32256.962	3099.2122	2.295E-03	7.9. 7E-22	2.650E+04	7.41410E-01	78
9.5	10.5	2019.633	-	0	0	2 1 1 0 .51	32261.029	3090.8150	3.295E-03	1.077E-22	2.650E+04	7.41410E-01	79
10.5	10.5	2019.633	-	0	0	1 1 1 0 .51	32263.426	3090.5856	9.153E-02	2.993E-21	6.230E+05	2.09700E+01	80
7.5	7.5	1368.720	-	0	0	2 2 1 7 .51	32281.659	3096.0392	3.354E+00	1.090E-19	6.340E+05	1.44631E+01	81
4.5	7.5	1368.720	-	0	0	1 2 1 7 .51	32283.579	3096.6512	1.776E-01	5.000E-21	2.991E+04	7.97604E-01	82
5.5	1.5	107.751	0	0	0	2 2 1 1 .51	32286.475	3096.3714	3.111E+02	1.017E-17	3.970E+05	1.10159E+00	83
1.5	1.5	107.751	0	0	0	1 2 1 1 .51	32286.827	3096.3196	4.100E+02	1.367E-17	2.667E+05	1.44900E+00	84
3.5	4.5	355.105	0	0	0	1 1 1 4 .51	32289.066	3096.1250	5.244E+02	1.719E-17	4.563E+05	5.12107E+00	85
0.5	9.5	1654.577	0	0	0	2 1 9 .51	32295.059	3095.5502	3.207E-02	1.049E-21	2.999E+04	7.45546E-01	86
9.5	9.5	1654.577	0	0	0	1 1 9 .51	32297.240	3095.3414	7.490E-01	2.449E-20	6.304E+05	1.09017E+01	88
6.5	6.5	1070.509	0	0	0	2 2 1 6 .51	32306.695	3096.6269	1.666E+01	5.443E-19	6.332E+05	1.21555E+01	89
7.5	6.5	1070.509	0	0	0	1 2 1 6 .51	32306.695	3096.4605	1.106E+00	3.014E-20	3.602E+04	0.99222E-01	90
5.5	5.5	126.449	-	0	0	1 2 1 .51	32314.091	3093.7271	5.435E+02	1.777E-17	6.010E+05	1.33333E+00	91
5.5	5.5	924.013	-	0	0	2 2 1 5 .51	32323.040	3092.7972	6.436E+01	2.105E-10	6.252E+05	1.00647E+01	92
6.5	5.5	924.013	-	0	0	1 2 1 5 .51	32325.320	3092.6524	5.512E+00	1.002E-19	4.509E+04	9.23700E-01	93
7.5	0.5	1324.291	-	0	0	2 1 8 .51	32326.047	3092.5020	2.544E-01	0.320E-21	3.702E+04	8.50667E-01	94
0.5	0.5	1324.291	-	0	0	1 1 8 .51	32329.067	3092.3952	4.907E+00	6.405E-19	6.347E+05	1.68236E+01	95
4.5	4.5	600.194	0	0	0	2 2 1 4 .51	32330.736	3091.3693	1.914E+02	6.406E-10	6.099E+05	4.50160E+00	96
5.5	4.5	600.194	0	0	0	1 2 1 4 .51	32343.020	3091.2466	2.177E+01	7.126E-19	5.777E+04	9.05130E-01	97
2.5	3.5	201.922	-	0	0	1 1 3 .51	32343.567	3091.1943	1.066E+03	3.407E-17	4.956E+05	4.11042E+00	98
5.5	5.5	126.291	0	0	0	2 2 1 .51	32347.934	3090.4902	5.466E+02	1.701E-17	4.026E+05	1.33333E+00	99
1.5	5.5	126.291	0	0	0	1 2 1 .51	32348.207	3090.4565	2.717E+02	0.006E-10	1.224E+05	6.66645E-01	100

Table 8 (Contd.)

J' J''	Lower energy vacuum cm ⁻¹	Transition	Frequency vacuum cm ⁻¹	Wavelength STP angstroms	Intensity cm ⁻² -atm ⁻¹	Intensity cm/molecule	Einstein sec ⁻¹	A Line strength	Number
T = 240 K									
3-5	429.275 -	0 0 2 21 3-51	32349.150	3090.3741	4.209E+02	1.40E-17	5.04E+05	6.52912E+00	101
4-5	429.275 -	0 0 1 21 3-51	32350.203	3090.2735	6.711E+01	2.19E-10	7.31E+04	1.02990E+00	102
6-5	1029.092 +	0 0 2 11 7-51	32356.112	3089.9001	1.641E+00	5.36E-20	4.65E+04	9.31010E-01	103
1-5	107.491 -	0 0 2 21 1-51	32356.410	3089.6717	7.776E+02	2.94E-17	4.97E+05	2.75253E+00	104
2-5	200.769 +	0 0 2 21 2-51	32356.501	3089.0553	6.904E+02	2.80E-17	5.46E+05	4.55550E+00	105
2-5	107.491 -	0 0 1 21 1-51	32356.997	3089.0156	2.637E+02	0.52E-10	1.12E+05	9.37233E-01	106
3-5	200.769 +	0 0 1 21 2-51	32355.401	3089.7770	1.571E+02	5.13E-10	9.22E+04	1.03070E+00	107
7-5	1029.092 +	0 0 1 11 7-51	32355.050	3089.7342	2.559E+01	0.36E-19	6.35E+05	1.47340E+01	108
5-5	769.216 -	0 0 2 11 6-51	32379.405	3087.4063	0.504E+00	2.00E-19	5.99E+04	1.01634E+00	109
6-5	769.216 -	0 0 1 11 6-51	32380.917	3087.3422	1.055E+02	3.45E-10	6.31E+05	1.26352E+01	110
1-5	83.719 +	0 0 1 11 2-51	32390.059	3086.3945	1.679E+03	5.40E-17	5.77E+05	3.10620E+00	111
4-5	544.009 +	0 0 2 11 5-51	32402.122	3085.3217	3.642E+01	1.19E-10	7.94E+04	1.11315E+00	112
5-5	544.009 +	0 0 1 11 5-51	32403.405	3085.1995	3.412E+02	1.11E-17	6.21E+05	1.05264E+01	113
1-5	126.449 -	0 0 2 21 -51	32415.652	3084.0520	2.721E+02	0.97E-10	1.21E+05	6.6664E-01	114
3-5	355.900 -	0 0 2 11 6-51	32422.526	3083.3000	1.250E+02	4.00E-10	1.10E+05	1.22124E+00	115
4-5	355.900 -	0 0 1 11 6-51	32423.579	3083.2790	0.5-1E+02	2.79E-17	6.02E+05	8.41497E+00	116
-5	0.000 -	0 0 1 11 1-51	32440.540	3081.6677	2.060E+03	6.73E-17	0.611E+05	2.35645E+00	117
2-5	202.370 +	0 0 2 11 3-51	32440.900	3081.6259	3.452E+02	1.12E-17	1.61E+05	1.33651E+00	118
3-5	202.370 +	0 0 1 11 3-51	32441.001	3081.5479	1.621E+03	5.30E-17	5.70E+05	6.31440E+00	119
2-5	107.751 +	0 0 2 21 1-51	32455.599	3080.2370	3.902E+02	1.30E-17	1.711E+05	1.41290E+00	120
1-5	83.920 -	0 0 2 11 2-51	32457.901	3080.0117	2.647E+02	2.50E-17	2.64E+05	1.45015E+00	121
2-5	83.920 -	0 0 1 11 2-51	32459.560	3079.9560	2.233E+03	7.30E-17	5.15E+05	4.25111E+00	122
-5	-0.56 +	0 0 2 11 1-51	32474.170	3078.4762	1.369E+03	4.47E-17	5.73E+05	1.56447E+00	123
1-5	-0.56 +	0 0 1 11 1-51	32474.523	3078.4420	1.961E+03	6.41E-17	4.10E+05	2.24021E+00	124
3-5	429.450 +	0 0 2 21 3-51	32489.304	3077.0346	3.472E+02	1.13E-17	2.65E+05	2.27273E+00	125
3-5	4371.365 -	0 0 2 21 3-51	32517.473	3074.3765	2.090E+02	6.04E-10	2.31E+05	3.20653E+00	126
15-5	4371.365 -	0 0 2 211 6-51	32531.710	3073.0310	4.205E-10	1.37E-27	2.65E+05	1.42637E+01	127
5-5	600.100 -	0 0 2 21 4-51	32540.433	3072.2072	9.300E+01	3.44E-10	1.40E+05	9.10173E+00	128
1-5	0.000 -	0 0 2 11 1-51	32541.901	3072.0606	0.575E+02	2.00E-17	1.03E+05	9.00002E-01	129
2-5	0.000 -	0 0 1 11 1-51	32542.400	3072.0131	5.771E+02	1.00E-17	0.801E+04	6.62664E-01	130
14-5	3041.676 +	0 0 2 211 3-51	32551.652	3071.1403	9.616E-07	3.44E-26	2.71E+05	1.12577E+01	131
6-5	024.525 +	0 0 2 21 5-51	32558.679	3070.4055	3.110E+01	1.01E-10	2.62E+05	5.17021E+00	132
2-5	83.719 +	0 0 2 21 2-51	32559.631	3070.3956	6.715E+02	2.19E-17	1.55E+05	1.27305E+00	133
3-5	83.719 +	0 0 1 11 2-51	32560.452	3070.3162	0.076E+02	2.64E-17	1.44E+05	1.54040E+00	134
15-5	4341.046 -	0 0 2 1015-51	32561.229	3070.2450	2.396E-09	7.03E-29	1.271E+04	6.77930E-01	135
13-5	3344.522 -	0 0 2 2112-51	32567.242	3069.6700	1.795E-05	5.07E-25	2.75E+05	1.22503E+01	136
7-5	1077.054 -	0 0 2 21 6-51	32572.405	3069.1040	0.056E+00	2.43E-19	2.71E+05	6.18407E+00	137
3-5	201.922 -	0 0 2 11 3-51	32576.504	3068.8053	3.474E+02	1.13E-17	1.22E+05	1.34301E+00	138
4-5	201.922 -	0 0 1 11 3-51	32577.557	3068.7061	6.475E+02	2.11E-17	1.031E+05	2.52505E+00	139
12-5	2000.525 +	0 0 2 2111-51	32570.555	3068.6120	2.721E-04	0.30E-24	2.70E+05	1.12410E+01	140

8.5	7.5	1367.617	•	R	2	20	7.51	32502.019	3060.2059	1.620E+00	5.32E-20	2.77E+05	7.19504E+00	161	
16.5	16.5	2010.759	•	R	0	2	1016.51	32502.570	3060.2339	6.237E-00	2.03E-27	1.64E+04	7.11104E-01	162	
11.5	10.5	2450.279	-	R	2	2110.51	32505.653	32505.653	3067.0436	3.337E-00	1.09E-22	2.01E+05	1.02315E+01	163	
15.5	14.5	3010.759	•	R	1	1016.51	32505.945	32505.945	3067.9126	1.140E-06	3.09E-26	2.61E+04	1.39600E+01	164	
9.5	8.5	1693.290	-	R	2	21	0.51	32507.372	3067.7010	2.596E-01	0.491E-21	2.04E+05	0.20015E+00	165	
10.5	9.5	2054.353	•	R	2	21	0.51	32508.503	3067.6670	3.290E-02	1.07E-21	2.01E+05	0.22020E+00	166	
4.5	4.5	355.105	•	R	0	2	11	6.51	32591.026	1.350E+02	6.41E-02	9.577E+04	1.31730E+00	167	
5.5	4.5	355.105	•	R	1	11	6.51	32593.109	3067.2410	3.615E+02	1.10E-17	2.13E+05	3.55940E+00	168	
13.5	13.5	3311.902	-	R	0	2	1013.51	32599.703	3066.6130	1.339E-06	6.37E-26	1.69E+04	7.40641E-01	169	
14.5	13.5	3311.902	-	R	1	1013.51	32603.023	32603.023	3066.1109	2.254E-35	7.37E-25	2.64E+04	1.29624E+01	170	
5.5	5.5	543.575	-	R	0	2	11	5.51	32625.046	6.111E+01	1.34E-10	7.52E+04	1.25104E+00	171	
6.5	5.5	543.575	-	R	1	11	5.51	32606.557	3065.9766	1.494E+02	4.90E-10	2.35E+05	6.41126E+00	172	
12.5	12.5	2446.009	•	R	0	2	1012.51	32612.991	3065.3710	2.345E-05	7.73E-25	1.97E+04	7.70527E-01	173	
6.5	6.5	767.150	•	R	0	2	11	6.51	32615.746	3.65.1120	9.965E+00	3.25E-10	5.90E+04	1.17227E+00	174
13.5	12.5	2046.009	•	R	1	11	6.51	32616.012	3065.0479	3.677E-04	1.137E-23	2.69E+05	1.19335E+01	175	
7.5	6.5	767.150	•	R	1	11	6.51	32617.646	3064.9492	6.754E-01	1.95E-10	2.50E+05	9.67107E+00	176	
11.5	11.5	2413.613	-	R	0	2	1011.51	32622.320	3064.4952	3.420E-04	1.11E-23	2.31E+04	0.30010E-01	177	
7.5	7.5	1026.730	-	R	0	2	11	7.51	32623.604	1.942E+00	6.35E-20	4.63E+04	1.09322E+00	178	
12.5	11.5	2413.613	-	R	1	1011.51	32625.137	32625.137	3064.2305	4.346E-03	1.421E-22	2.71E+05	1.09640E+01	179	
8.5	7.5	1026.730	-	R	1	11	7.51	32625.569	3064.1900	1.176E+01	3.04E-19	2.60E+05	6.72652E+00	180	
10.5	10.5	2015.036	•	R	0	2	1010.51	32627.901	3063.9710	4.65E-03	1.32E-22	2.74E+04	0.91564E-01	181	
8.5	8.5	1321.252	•	R	0	2	11	8.51	32629.304	3063.9256	3.055E-01	9.90E-21	3.95E+04	1.01913E+00	182
9.5	9.5	1650.790	-	R	1	2	11	8.51	32629.472	3063.7054	3.044E-02	1.27E-21	3.27E+04	0.41013E-01	183
11.5	10.5	2015.036	•	R	1	11	8.51	32630.510	3063.7266	6.300E-02	1.43E-21	2.72E+05	9.06003E+00	184	
9.5	8.5	1321.252	•	R	1	11	8.51	32633.565	3063.7280	2.293E+00	7.49E-20	2.67E+05	7.7050E+00	185	
10.5	9.5	1650.790	-	R	1	11	9.51	32632.269	3063.5600	3.545E-01	1.15E-20	2.70E+05	0.02700E+00	186	
2.5	1.5	83.920	-	S	2	11	1.51	32643.295	3062.5260	1.636E+02	5.34E-10	2.30E+04	1.07007E-01	187	
3.5	2.5	83.920	-	S	2	11	2.51	32644.505	3057.7289	1.570E+02	5.13E-10	2.74E+04	2.94634E-01	188	
4.4	3.5	202.370	•	S	2	11	3.51	32744.561	3053.5544	0.567E+01	2.33E-10	2.56E+04	3.40030E-01	189	
5.5	4.5	355.980	-	S	2	11	4.51	32792.722	3048.5704	3.695E+01	1.20E-10	2.22E+04	3.63319E-01	190	
6.5	5.5	544.009	•	S	2	11	5.51	32830.355	3046.3101	1.160E+01	3.01E-19	1.07E+04	3.59494E-01	191	
7.4	6.5	769.216	-	S	2	11	6.51	32881.122	3046.3740	2.905E+00	9.49E-26	1.56E+04	3.47219E-01	192	
8.5	7.5	1029.092	•	S	2	11	7.51	32920.546	3036.7331	5.74E-01	1.00E-20	1.31E+04	3.31653E-01	193	
9.5	8.5	1324.291	-	S	2	11	8.51	32956.371	3033.4317	9.217E-02	3.01E-21	1.11E+04	3.19300E-01	194	
10.5	9.5	1656.577	•	S	2	11	9.51	32980.363	3030.4901	1.109E-02	3.00E-22	9.44E+03	2.99663E-01	195	
11.5	10.5	2019.633	-	S	2	1010.51	33016.273	33016.273	3027.9254	1.245E-03	4.07E-23	0.14E+03	2.05026E-01	196	
12.5	11.5	2419.001	•	S	2	1011.51	33039.999	33039.999	3025.7534	1.061E-04	3.17E-24	7.03E+03	2.71673E-01	197	
13.5	12.5	2052.495	-	S	2	1012.51	33059.200	33059.200	3023.0407	7.377E-06	2.41E-25	6.10E+03	2.59626E-01	198	
14.5	13.5	3319.355	•	S	2	1013.51	33073.974	33073.974	3322.6451	4.200E-07	1.33E-26	5.33E+03	2.40029E-01	199	
15.5	14.5	3019.156	-	S	2	1014.51	33093.914	33093.914	3021.7365	1.965E-08	6.42E-20	4.60E+03	2.39107E-01	200	

THE INTEGRATED INTENSITY FOR THE BAND IS 2.79400E+04 CM-2 ATM-1 AT T = 240.0 K OR 9.13039E-16 CM/MOLECULE

Table 9. Line parameters for the $A^1\Sigma-X^1\Pi(0,0)$ OH band at 4607K.

J'	J''	Lower energy vacuum cm^{-1}	Transition	Frequency vacuum cm^{-1}	Wavelength STP angstroms	Intensity $\text{cm}^{-2}\text{-atm}^{-1}$	Intensity $\text{cm}/\text{molecule}$	Einstein sec^{-1}	A Line strength	Number
39.5	46.5	26949.529	0 P 1 2140.51	27339.521	3656.669	3.209E-06	2.01E-24	6.67E+01	1.5670E-01	1
39.5	39.5	25000.074	0 P 1 2139.51	27530.904	3631.2340	6.34E-06	3.97E-24	9.70E+01	1.5329E-01	2
37.5	30.5	24796.104	0 P 1 2138.51	27716.057	3606.0030	1.15E-05	7.17E-24	1.31E+02	1.5232E-01	3
36.5	37.5	23770.737	0 P 1 2137.51	27897.476	3583.5300	1.959E-05	1.22E-23	1.677E+02	1.5157E-01	4
35.5	36.5	22604.637	0 P 1 2136.51	28073.156	3561.1017	3.20E-05	2.02E-23	2.07E+02	1.5102E-01	5
35.5	35.5	21646.080	0 P 1 2135.51	28246.107	3537.5400	5.10E-05	3.24E-23	2.50E+02	1.5072E-01	6
39.5	40.5	24910.107	0 P 2 2140.51	28257.590	3537.0601	0.005E-04	5.54E-22	1.95E+04	4.0972E-01	7
40.5	40.5	26910.107	0 P 2 2140.51	28263.694	3537.0970	7.11E-06	4.46E-24	1.52E+02	4.2909E-01	8
33.5	34.5	20222.193	0 P 1 2134.51	28410.042	3510.7769	0.10E-05	5.07E-23	2.95E+02	1.5040E-01	9
30.5	39.0	25037.352	0 P 2 2139.51	28445.624	3514.4761	1.72E-03	1.03E-21	2.01E+04	3.3902E-01	10
39.5	39.5	25037.352	0 P 1 2139.51	28451.090	3513.7239	1.65E-05	1.03E-23	2.62E+02	5.2673E-01	11
39.5	46.5	25010.569	0 P 1 2140.51	28470.401	3511.4057	1.20E-03	7.96E-22	2.80E+04	4.1162E-01	12
32.5	33.5	19611.744	0 P 1 2133.51	28573.369	3490.7612	1.25E-04	7.05E-23	3.40E+02	1.5001E-01	13
37.5	30.5	24766.199	0 P 2 2130.51	28626.016	3492.2200	3.05E-03	1.91E-21	3.70E+04	3.0991E-01	14
30.5	30.5	24766.199	0 P 1 2130.51	28632.060	3491.4916	3.23E-05	2.02E-23	3.02E+02	5.2495E-01	15
30.5	39.5	24767.204	0 P 1 2139.51	28651.775	3489.1046	2.45E-03	1.53E-21	2.00E+04	4.0150E-01	16
31.5	32.5	18610.524	0 P 1 2127.51	28732.000	3479.4466	1.90E-04	1.19E-22	4.04E+02	1.5122E-01	17
36.5	37.5	23705.526	0 P 2 2137.51	28801.537	3471.0466	5.17E-03	3.20E-21	4.62E+02	3.0001E-01	18
37.5	37.5	23705.526	0 P 1 2137.51	28807.515	3470.3227	5.05E-05	3.03E-23	5.11E+02	5.2300E-01	19
37.5	30.5	23600.672	0 P 1 2130.51	28826.569	3460.0208	4.34E-03	2.71E-21	3.00E+04	3.9165E-01	20
30.5	31.5	17637.220	0 P 1 2131.51	28806.947	3460.7799	2.07E-04	1.00E-22	4.67E+02	1.5195E-01	21
35.5	36.5	22656.237	0 P 2 2136.51	28970.010	3450.0567	0.23E-03	5.16E-21	5.50E+04	3.7000E-01	22
36.5	36.5	22656.237	0 P 1 2136.51	28975.976	3450.1463	9.00E-05	6.19E-23	6.51E+02	5.2320E-01	23
36.5	37.5	22637.036	0 P 1 2137.51	28995.177	3447.0615	7.20E-03	4.53E-21	4.74E+04	3.0176E-01	24
29.5	30.5	16075.095	0 P 1 2130.51	29030.402	3442.7290	4.20E-04	2.60E-22	5.30E+02	1.5207E-01	25
40.5	40.5	26949.529	0 P 2 2140.51	29120.465	3433.0269	1.10E-03	7.00E-22	2.57E+04	0.1457E-01	26
34.5	35.5	21619.256	0 P 2 2135.51	29132.621	3431.5044	1.20E-02	0.07E-21	6.56E+04	3.6015E-01	27
35.5	35.5	21619.256	0 P 1 2135.51	29138.537	3430.0977	1.67E-04	1.01E-22	6.04E+02	5.2342E-01	28
35.5	36.5	21599.090	0 P 1 2136.51	29157.024	3420.6199	1.60E-02	7.26E-21	5.71E+04	3.7107E-01	29
20.5	29.5	15731.331	0 P 2 2134.51	29186.542	3425.2555	6.31E-04	3.96E-22	6.10E+02	1.5412E-01	30
33.5	34.5	20595.523	0 P 2 2139.51	29209.616	3413.2004	1.95E-02	1.22E-20	7.53E+04	5.5022E-01	31
34.5	34.5	20595.523	0 P 1 2134.51	29295.473	3412.5177	2.50E-04	1.62E-22	9.67E+02	5.2425E-01	32
39.5	39.5	25040.074	0 Q 2 2139.51	29307.631	3411.1921	2.55E-03	1.59E-21	4.30E+04	7.9463E-01	33
40.5	39.5	25040.074	0 Q 1 2139.51	29313.727	3410.3927	6.32E-06	3.95E-24	1.00E+02	2.9511E-01	34
34.5	35.5	20575.990	0 P 1 2135.51	29316.990	3410.2440	1.41E-02	1.13E-20	6.72E+04	3.6197E-01	35
39.5	40.5	25495.390	0 P 2 2140.51	29323.316	3409.6283	1.10E-05	6.93E-24	1.07E+02	3.5270E-01	36
40.5	40.5	25495.390	0 Q 1 2140.51	29326.412	3409.9175	1.50E-03	9.92E-22	2.62E+04	0.1357E-01	37
27.5	28.5	14006.007	0 P 1 2120.51	29331.526	3400.7231	9.21E-04	5.77E-22	7.05E+02	1.5560E-01	38
32.5	33.5	19505.991	0 P 2 2133.51	29441.240	3395.0205	2.94E-02	1.04E-20	0.59E+04	3.4020E-01	39
33.5	33.5	19505.991	0 P 1 2133.51	29447.044	3394.9522	4.03E-04	2.53E-22	1.54E+03	5.2579E-01	40
33.5	34.5	19566.207	0 P 1 2134.51	29466.747	3392.6022	2.73E-02	1.71E-20	7.71E+04	3.5207E-01	41
26.5	27.5	13000.997	0 Q 2 2127.51	29473.450	3391.9049	1.32E-03	0.02E-22	0.02E+02	1.5700E-01	42
30.5	30.5	24796.104	0 Q 2 2130.51	29406.793	3390.3755	4.04E-03	3.05E-21	6.15E+04	7.7460E-01	43
35.5	36.5	24796.104	0 R 1 2130.51	29492.066	3389.6774	1.39E-05	0.76E-24	1.72E+02	2.9570E-01	44
30.5	39.5	24703.345	0 P 2 2139.51	29499.632	3380.0939	2.19E-05	1.37E-23	2.76E+02	3.5257E-01	45
30.5	30.5	24703.345	0 Q 1 2139.51	29505.745	3380.2023	3.52E-03	2.25E-21	4.41E+04	7.9361E-01	46
31.5	32.5	18591.624	0 P 2 2132.51	29507.766	3370.0956	4.32E-02	2.71E-20	9.64E+04	3.3030E-01	47

32.5	32.5	10591.624	0	0	1	2132.53	29593.600	3170.1514	6.221E-04	3.099E-22	1.345E+03	5.20099E-01	69
25.5	26.5	13016.966	0	0	1	2126.53	29612.505	3175.0730	1.902E-03	1.182E-21	9.140E+02	1.50034E-01	69
32.5	33.5	10571.723	0	0	1	1133.53	29613.306	3175.0037	4.005E-02	2.940E-20	0.790E+04	1.62172E-01	69
37.5	37.5	23734.737	0	0	2	2137.53	29650.270	3170.7716	0.534E-03	5.349E-21	0.040E+04	7.94729E-01	51
30.5	37.5	23736.737	0	0	0	1	2137.53	3170.0049	2.605E-05	1.603E-23	2.467E+02	2.90017E-01	52
37.5	30.5	23721.729	0	0	2	1130.53	29671.206	3169.2939	3.074E-05	2.074E-23	3.730E+02	1.52042E-01	53
30.5	30.5	23721.729	0	0	0	1	1130.53	3160.6077	6.050E-03	4.293E-21	6.270E+04	7.79674E-01	54
30.5	31.5	17613.392	0	0	2	2131.53	29729.391	3162.7004	9.407E-02	3.940E-20	1.079E+05	3.20302E-01	55
31.5	31.5	17613.392	0	0	0	1	2131.53	3162.6699	9.407E-04	5.934E-22	1.569E+03	5.31100E-01	56
24.5	25.5	12155.073	0	0	1	2125.53	29740.962	3160.5030	2.691E-03	1.647E-21	1.030E+03	1.82469E-01	57
31.5	32.5	17593.790	0	0	1	1132.53	29755.140	3159.7905	5.961E-02	3.709E-20	9.060E+04	3.32260E-01	58
36.5	36.5	22604.637	0	0	2	2136.53	29822.396	3152.2211	1.416E-02	0.077E-21	9.970E+04	7.14762E-01	59
37.5	36.5	22604.637	0	0	0	1	2136.53	3151.5459	6.775E-05	2.933E-23	3.277E+02	2.90234E-01	60
36.5	37.5	22671.646	0	0	2	1137.53	29935.573	3150.7196	6.014E-05	4.270E-23	4.709E+02	3.53513E-01	61
37.5	37.5	22671.646	0	0	0	1	1137.53	3150.0644	1.196E-02	7.694E-21	0.100E+04	7.53735E-01	62
29.5	30.5	11692.271	0	0	2	2130.53	29866.335	3147.2091	9.002E-02	5.643E-20	1.100E+05	3.10420E-01	63
30.5	30.5	11692.271	0	0	0	1	2130.53	3146.6661	1.421E-03	0.900E-22	1.017E+03	5.39119E-01	64
23.5	24.5	11315.663	0	0	1	2124.53	29802.546	3145.4732	3.703E-03	2.371E-21	1.170E+03	1.65919E-01	65
30.5	31.5	11631.946	0	0	1	1131.53	29832.221	3144.3904	0.645E-02	5.419E-20	1.170E+05	3.22394E-01	66
35.5	35.5	21646.000	0	0	2	2135.53	29979.629	3134.6604	2.263E-02	1.410E-20	4.169E+02	7.16791E-01	67
36.5	35.5	21646.000	0	0	0	1	2135.53	3133.9970	0.091E-05	5.070E-23	4.169E+02	3.00054E-01	68
35.5	36.5	21633.910	0	0	2	1136.53	29992.029	3133.1716	1.126E-04	7.095E-23	5.930E+02	3.56011E-01	69
20.5	29.5	13709.237	0	0	2	2129.53	29990.795	3132.5090	1.277E-02	1.290E-20	1.300E+05	3.00440E-01	70
36.5	36.5	21633.910	0	0	0	1	1136.53	3132.5090	1.975E-02	1.290E-20	1.300E+05	3.00440E-01	71
29.5	29.5	15709.237	0	0	0	1	2129.53	3131.9017	2.100E-03	1.320E-21	2.092E+03	5.39924E-01	72
22.5	23.5	10500.267	0	0	0	1	2123.53	3130.0644	5.250E-03	3.290E-21	1.339E+03	1.65913E-01	73
29.5	30.5	15600.670	0	0	1	1130.53	30024.026	3129.6194	1.231E-01	7.717E-20	1.230E+05	3.12430E-01	74
27.5	28.5	16705.263	0	0	2	2120.53	30126.944	3110.3330	1.777E-01	1.114E-19	1.627E+05	2.90460E-01	75
34.5	34.5	20622.193	0	0	2	2134.53	30129.604	3110.0112	3.497E-02	2.192E-20	1.399E+05	6.04013E-01	76
20.5	20.5	14745.263	0	0	1	2120.53	30122.310	3117.7420	3.090E-03	1.937E-21	2.397E+03	5.55670E-01	77
35.5	36.5	20622.193	0	0	0	1	2134.53	3117.7420	1.313E-04	0.227E-23	5.000E+02	3.02297E-01	78
34.5	35.5	20604.204	0	0	2	1135.53	30142.147	3116.6592	7.252E-03	4.560E-21	1.517E+03	1.73000E-01	79
23.5	29.5	14764.634	0	0	0	1	1129.53	3115.6502	1.733E-01	1.000E-19	1.330E+05	3.02505E-01	80
40.5	39.5	29437.952	0	0	2	2134.53	30232.641	3106.7313	0.706E-04	5.657E-22	1.529E+04	3.91494E-01	81
26.5	27.5	13001.320	0	0	2	2127.53	30250.955	3104.7292	2.442E-01	1.590E-19	1.549E+05	2.00479E-01	84
40.5	40.5	25010.569	0	0	2	1160.53	30251.424	3104.6761	0.926E-06	5.599E-24	1.550E+02	4.39490E-01	85
27.5	27.5	13001.320	0	0	0	1	2127.53	3103.291	3.144E-02	1.970E-20	1.210E+05	7.13303E-01	86
20.5	21.5	0794.563	0	0	1	2121.53	30256.213	3102.0425	9.090E-03	6.204E-21	1.720E+03	1.77544E-01	87
33.5	33.5	19611.744	0	0	2	2132.53	30273.392	3102.2600	5.206E-02	3.313E-20	1.599E+05	6.74027E-01	89
27.5	20.5	13060.205	0	0	1	1120.53	30277.329	3101.0506	2.402E-01	1.504E-19	1.459E+05	2.92574E-01	90
34.5	33.5	19611.744	0	0	0	1	2133.53	3101.6409	2.099E-04	1.319E-22	6.162E+02	3.04904E-01	91
33.5	34.5	19597.902	0	0	2	1134.53	30207.234	3100.7707	4.030E-04	1.773E-22	0.521E+02	3.50169E-01	92
25.5	26.5	12990.371	0	0	0	1	1134.53	30203.374	3.321E-01	3.032E-26	1.609E+05	6.91064E-01	93
26.5	26.5	12990.371	0	0	0	1	2126.53	30370.901	3.321E-01	2.000E-19	1.609E+05	2.70470E-01	93
26.5	26.5	12990.371	0	0	0	1	2126.53	3291.1113	6.430E-03	4.030E-21	3.113E+03	5.60204E-01	94
19.5	20.5	0206.027	0	0	1	2120.53	30391.910	3209.4009	1.341E-02	0.499E-21	1.960E+03	1.92606E-01	95
26.5	27.5	12976.043	0	0	1	1127.53	35397.552	3290.7912	2.090E-01	2.090E-19	1.500E+05	2.02630E-01	96
39.5	30.5	21766.199	0	0	2	2130.53	30459.507	3207.4903	1.070E-03	1.197E-21	2.449E+04	3.16090E-01	97
32.5	32.5	10616.429	0	0	2	2132.53	30410.009	3207.3574	7.065E-02	4.930E-20	1.010E+05	6.50032E-01	98
33.5	32.5	10616.429	0	0	0	1	2132.53	3246.7310	6.207E-04	2.000E-22	7.363E+02	3.00167E-01	99
32.5	32.5	10602.331	0	0	2	1133.53	30424.950	3205.0341	4.302E-04	2.707E-22	1.609E+03	3.60670E-01	100

Table 3 (Contd.)

J' J''	Lower energy vacuum cm ⁻¹	Transition	Frequency vacuum cm ⁻¹	Wavelength STP angstroms	Intensity cm ⁻² atm ⁻¹	Intensity cm/molecule	Einstein sec ⁻¹	A Line strength	Number
39.5 39.5	26747.204	0 0 2 1039.50	30420.421	3205.4547	2.049E-05	1.29E-23	2.674E-02	6.30270E-01	101
33.5 33.5	16002.331	0 0 1 1033.50	30430.703	3205.2003	7.276E-02	4.56E-20	1.620E-05	6.73094E-01	102
40.5 39.5	24797.204	0 0 1 1039.50	30436.517	3206.7966	1.220E-03	7.69E-22	1.950E-06	1.90114E-01	103
26.5 26.5	12137.370	0 0 2 2025.50	30487.162	3270.1242	4.449E-01	2.70E-19	1.700E-05	2.60466E-01	104
25.5 25.5	12137.370	0 0 1 2025.50	30492.102	3270.5044	9.134E-01	5.72E-21	3.539E-03	5.69307E-01	105
18.5 19.5	7494.040	0 0 1 2019.50	30513.229	3276.3229	1.001E-02	1.12E-20	2.237E-03	1.00501E-01	106
25.5 26.5	12135.590	0 0 1 1026.50	30513.954	3276.2450	4.433E-01	2.77E-19	1.704E-05	2.72094E-01	107
31.5 31.5	17337.220	0 0 2 2031.50	30542.169	3273.2103	1.154E-01	7.23E-20	2.031E-05	6.34027E-01	108
32.5 31.5	17637.220	0 0 1 2031.50	30547.093	3272.6049	5.077E-04	3.10E-22	9.670E-02	3.11010E-01	109
31.5 32.5	17622.044	0 0 2 1032.50	30556.545	3271.6703	6.662E-04	4.17E-22	1.170E-03	3.63711E-01	110
32.5 32.5	17622.044	0 0 1 1032.50	30562.569	3271.0655	1.977E-01	6.75E-20	1.034E-05	6.53013E-01	111
30.5 37.5	23705.526	0 0 2 2037.50	30577.451	3269.4413	3.494E-03	2.19E-21	3.303E-04	1.71711E-01	112
30.5 30.5	23086.472	0 0 2 1030.50	30596.505	3267.4052	4.030E-05	2.53E-23	3.007E-02	4.37905E-01	113
23.5 24.5	11299.250	0 0 2 2024.50	30599.620	3267.0717	5.991E-01	3.69E-19	1.914E-05	2.50442E-01	114
39.5 30.5	23606.472	0 0 1 1030.50	30602.570	3266.7560	2.640E-03	1.65E-21	2.470E-04	1.00211E-01	115
24.5 24.5	11299.250	0 0 1 2024.50	30606.517	3266.5490	1.006E-02	0.06E-21	4.012E-03	5.79603E-01	116
24.5 25.5	11277.107	0 0 1 1025.50	30626.660	3266.1072	5.096E-01	3.69E-19	1.079E-05	2.62745E-01	117
17.5 10.5	6011.055	0 0 1 2010.50	30632.193	3263.5944	2.390E-02	1.50E-20	2.557E-03	1.95070E-01	118
30.5 30.5	16075.095	0 0 2 2030.50	30667.609	3259.0209	1.664E-01	1.04E-19	2.259E-05	6.14030E-01	119
31.5 36.5	16075.095	0 0 1 2030.50	30673.339	3259.2200	7.723E-04	4.04E-22	1.014E-03	1.16007E-01	120
30.5 31.5	16660.417	0 0 2 1031.50	30682.365	3258.2614	1.002E-03	6.20E-22	1.355E-03	3.67300E-01	121
31.5 31.5	16660.417	0 0 1 1031.50	30680.012	3257.6619	1.571E-01	9.01E-19	2.035E-05	6.33027E-01	122
22.5 23.5	10006.962	0 0 2 2023.50	30700.495	3255.4090	7.609E-01	4.01E-19	2.035E-05	2.64044E-01	123
23.5 23.5	10006.962	0 0 1 2023.50	30713.247	3254.9053	1.792E-02	1.12E-20	4.544E-03	5.91202E-01	124
23.5 26.5	10662.394	0 0 1 2024.50	30735.016	3252.5951	7.760E-01	4.06E-19	1.957E-05	2.52707E-01	125
37.5 36.5	22656.237	0 0 2 2026.50	30736.770	3252.4933	6.023E-03	3.77E-21	4.350E-04	1.61013E-01	126
16.5 17.5	6157.034	0 0 1 2017.50	30740.024	3251.2191	3.162E-02	1.90E-20	2.932E-03	2.02609E-01	127
37.5 37.5	22637.036	0 0 2 1037.50	30755.979	3250.4627	7.231E-05	4.53E-23	5.190E-02	6.37631E-01	128
30.5 37.5	22637.036	0 0 1 1037.50	30762.023	3249.0240	4.890E-03	3.07E-21	3.633E-04	1.70303E-01	129
29.5 29.5	15731.031	0 0 2 2029.50	30787.575	3247.1267	2.366E-01	1.40E-19	2.600E-05	5.44794E-01	130
30.5 29.5	15731.031	0 0 1 2029.50	30793.136	3246.5403	1.162E-03	9.33E-22	1.194E-03	1.20775E-01	131
29.5 36.5	15716.026	0 0 2 1030.50	30802.500	3246.5449	1.809E-03	7.30E-22	1.564E-03	3.71602E-01	132
30.5 30.5	15716.026	0 0 1 1030.50	30800.161	3246.9591	2.754E-01	1.61E-19	2.207E-05	6.13021E-01	133
21.5 22.5	9695.394	0 0 2 2022.50	30810.069	3244.3550	9.916E-01	6.21E-19	2.157E-05	2.30351E-01	134
22.5 22.5	9695.394	0 0 1 2022.50	30810.477	3243.0707	2.672E-02	1.54E-20	5.144E-03	6.04507E-01	135
22.5 23.5	9672.362	0 0 1 1023.50	30841.509	3241.4401	1.006E-00	6.30E-19	2.002E-05	2.42023E-01	136
15.5 16.5	5533.620	0 0 1 2016.50	30863.123	3239.1700	4.139E-02	2.59E-20	3.300E-03	2.10069E-01	137
36.5 35.5	21619.256	0 0 2 2035.50	30887.777	3236.5925	9.640E-03	6.10E-21	5.343E-04	1.51911E-01	138
20.5 20.5	14006.007	0 0 2 2020.50	30905.022	3235.1005	3.317E-01	2.07E-19	2.723E-05	5.74761E-01	139
36.5 36.5	21599.090	0 0 2 1036.50	30907.135	3234.5653	1.220E-04	7.69E-23	6.620E-02	4.37023E-01	140
29.5 20.5	14006.007	0 0 1 2020.50	30907.409	3234.5242	1.722E-03	1.07E-21	1.367E-03	3.26157E-01	141
37.5 36.5	21599.090	0 0 1 1036.50	30913.143	3233.9366	0.396E-03	5.26E-21	4.004E-04	1.60390E-01	142
20.5 21.5	9331.446	0 0 2 2021.50	30915.046	3233.6530	1.260E-00	7.00E-19	2.274E-05	2.20203E-01	143
20.5 29.5	17790.447	0 0 2 1029.50	30917.303	3233.6931	2.193E-03	1.37E-21	1.794E-03	3.76297E-01	144
21.5 21.5	9331.446	0 0 1 2021.50	30923.303	3233.1077	3.302E-02	2.12E-20	5.037E-03	6.19413E-01	145
29.5 29.5	17790.447	0 0 1 1029.50	30922.050	3232.9214	3.105E-01	1.99E-19	2.519E-05	5.93101E-01	146

21.5	22.5	0907.090	0	1	1022.50	3093.051	3230.7272	1.200E+00	0.074E-19	2.200E+05	2.32050E+01	167
16.5	19.5	0939.082	0	0	1 2115.50	36375.003	3227.6696	5.360E-02	2.364E-20	3.910E+03	2.29341E-01	168
27.5	27.5	13900.997	0	0	2 2127.50	31011.210	3223.7096	6.507E-01	7.079E-19	2.960E+05	3.56716E+01	169
19.5	20.5	0193.990	0	0	2 2120.50	31010.510	3223.3665	1.501E+00	9.960E-19	2.390E+05	2.10190E+01	150
20.5	27.5	13900.997	0	0	1 2127.50	31010.576	3223.1510	2.530E-03	2.360E-21	1.570E+03	3.32200E-01	151
20.5	20.5	0193.990	0	0	1 2120.50	31010.089	3222.9190	6.503E-02	2.073E-20	6.610E+03	6.36194E-01	152
27.5	20.5	13005.249	0	0	2 1020.50	31025.957	3222.6733	3.100E-03	1.990E-21	2.040E+03	3.01794E-01	153
35.5	34.5	20595.523	0	0	2 1026.50	31030.725	3221.6921	1.542E-01	6.060E-21	6.200E+06	3.22000E+01	154
20.5	20.5	13005.249	0	0	1 1020.50	31032.324	3221.5161	4.435E-01	2.700E-19	2.750E+05	5.73000E+01	155
20.5	21.5	0109.066	0	0	1 1021.50	31002.933	3220.6151	1.624E+00	1.010E-10	2.330E+05	2.22000E+01	156
35.5	35.5	20575.990	0	0	2 1035.50	31050.250	3219.0567	2.012E-06	1.020E-22	0.100E+02	6.30993E-01	157
13.5	14.5	0377.319	0	0	1 2016.50	31006.603	3216.0096	6.095E-02	4.322E-20	4.540E+03	2.31060E-01	159
10.5	19.5	7403.075	0	0	2 2019.50	31109.936	3213.0700	1.956E+00	1.224E-10	2.510E+05	2.00093E+01	160
19.5	19.5	7403.075	0	0	1 2019.50	31116.070	3213.0519	6.153E-02	3.050E-20	7.510E+03	6.55405E-01	161
26.5	21.5	13016.966	0	0	2 2026.50	31115.369	3212.9239	6.249E-01	3.910E-19	3.130E+05	5.36660E+01	162
27.5	26.5	13016.966	0	0	1 2026.50	31120.567	3212.3011	3.677E-03	2.300E-21	1.010E+03	3.30950E-01	163
26.5	27.5	13000.797	0	0	2 1027.50	31131.670	3211.2551	6.570E-03	2.070E-21	2.300E+03	3.00027E-01	164
27.5	27.5	13000.797	0	0	1 1027.50	31136.736	3210.7120	6.693E-01	3.010E-19	2.991E+05	5.33054E+01	165
19.5	20.5	7659.105	0	0	1 1020.50	31130.079	3210.6962	2.022E+00	1.200E-10	2.640E+05	2.12070E+01	166
34.5	33.5	19565.991	0	0	2 2033.50	31165.006	3207.7097	2.371E-02	1.400E-20	7.310E+04	3.32094E+01	167
34.5	36.5	19566.207	0	0	2 1036.50	31105.509	3205.6036	3.195E-06	2.002E-22	9.010E+02	6.60700E-01	169
35.5	36.5	19566.207	0	0	1 1036.50	31191.565	3205.0749	2.130E-02	1.390E-20	6.360E+06	3.60540E+01	169
12.5	13.5	3046.059	0	0	1 2013.50	31191.092	3205.0352	0.799E-02	5.510E-20	5.320E+03	2.63203E-01	170
17.5	10.5	6001.926	0	0	2 2010.50	31202.100	3203.9776	2.306E+00	1.690E-10	2.630E+05	1.09960E+01	171
10.5	10.5	6901.026	0	0	1 2010.50	31206.151	3203.5707	0.174E-02	5.120E-20	5.540E+03	6.76291E-01	172
25.5	25.5	12154.073	0	0	2 2025.50	31216.479	3202.7159	0.406E-01	5.260E-19	3.420E+05	5.16590E+01	173
26.5	25.5	12154.073	0	0	1 2025.50	31219.622	3202.1006	5.270E-03	3.300E-21	2.070E+03	3.66490E-01	176
25.5	26.5	12130.246	0	0	2 1026.50	31231.100	3201.0106	6.527E-03	4.690E-21	2.650E+03	3.9500E-01	175
10.5	19.5	0776.031	0	0	1 1019.50	31231.666	3200.9555	2.400E+00	1.550E-10	3.220E+05	2.02076E+01	177
26.5	26.5	12130.246	0	0	1 1026.50	31236.251	3200.6036	9.264E-01	5.107E-19	3.220E+05	5.33000E+01	177
40.5	39.5	26703.165	0	5	2 1039.50	31206.649	3195.3279	5.912E-06	3.700E-26	7.970E+01	1.06740E-01	179
16.5	17.5	6100.942	0	0	2 2017.50	31291.320	3196.0509	2.065E-09	1.790E-10	2.740E+05	1.79010E+01	179
33.5	32.5	10501.024	0	0	2 2032.50	31293.513	3196.6270	3.563E-02	2.230E-20	0.361E+06	3.22100E+01	180
17.5	17.5	6100.942	0	0	1 2017.50	31295.166	3196.6644	1.070E-01	6.754E-20	9.740E+03	7.00104E-01	181
11.5	12.5	3340.000	0	0	1 2012.50	31296.666	3196.3051	1.112E-01	6.973E-20	6.200E+03	2.56973E-01	182
24.5	24.5	13315.603	0	0	2 2024.50	31300.069	3193.6600	1.117E+00	7.000E-19	3.660E+05	6.45500E+01	183
33.5	33.5	10571.720	0	0	2 1033.50	31313.400	3192.5972	4.970E-06	3.110E-22	1.161E+03	6.40073E-01	184
24.5	24.5	13315.603	0	0	1 2026.50	31313.099	3192.5401	7.519E-03	2.040E-26	7.390E+04	3.10415E+01	194
34.5	31.5	10571.720	0	0	1 1033.50	31319.264	3191.9990	3.250E-02	1.000E-10	2.700E+05	1.92064E+01	187
17.5	10.5	6122.320	0	0	1 1010.50	31321.421	3191.7904	3.007E+00	5.750E-19	3.020E+03	6.02060E-01	184
24.5	25.5	13290.532	0	0	2 1025.50	31326.010	3191.3130	9.107E-03	5.750E-21	3.660E+05	5.13740E+01	189
25.5	25.5	13290.532	0	0	1 1025.50	31331.020	3190.0925	1.101E+00	6.900E-19	3.660E+05	5.13740E+01	189
15.5	16.5	5525.697	0	0	2 2016.50	31377.379	3106.0041	3.394E+00	2.120E-19	2.057E+05	1.69662E+01	190
16.5	16.5	5525.697	0	0	1 2016.50	31300.901	3105.7223	1.400E-01	0.124E-20	1.110E+06	7.27041E-01	191
23.5	23.5	10500.267	0	0	2 2023.50	31300.619	3103.3327	1.663E+00	9.160E-19	3.090E+05	6.74000E+01	192
10.5	11.5	2944.110	0	0	1 2011.50	31300.969	3103.0992	1.395E-01	0.740E-26	7.600E+03	2.72600E-01	193
24.5	23.5	10500.267	0	0	1 2023.50	3164.520	3103.6370	1.057E-02	6.640E-21	2.700E+03	3.64211E-01	196
10.5	17.5	5690.652	0	0	1 1017.50	31600.225	3102.9508	3.506E+00	2.260E-10	2.020E+05	1.02060E+01	195
32.5	31.5	16163.392	0	0	2 2031.50	31613.067	3102.3092	5.267E-02	3.391E-20	9.650E+04	5.12260E+01	196
23.5	24.5	10402.500	0	0	1 1026.50	31616.299	3102.1639	1.204E-02	0.400E-21	3.690E+03	6.11015E-01	197
24.5	24.5	10402.500	0	0	2 1026.50	31621.107	3101.6657	1.552E+00	9.100E-19	3.690E+03	6.11015E-01	197
32.5	32.5	17593.790	0	0	2 1032.50	31633.969	3103.3648	7.620E-06	4.700E-22	1.360E+03	6.66160E-01	199
33.5	32.5	17593.790	0	0	1 1032.50	31639.766	3179.7677	4.069E-02	3.050E-20	0.030E+06	3.20670E+01	200

Table 9 (Contd.).

J' J''	Lower energy vacuum cm ⁻¹	Transition	Frequency vacuum cm ⁻¹	Wavelength STP angstroms	Intensity cm ⁻² atm ⁻¹	Intensity cm/molecule	Einstein A sec ⁻¹	Line strength	Number
39.5 30.5	23721.729	S R 2 1030.51	31533.976	3170.3269	1.292E-05	0.100E-24	1.25E+02	1.0309E-01	201
14.5 15.5	4932.933	P R 2 2015.51	31460.396	3177.6003	3.953E-00	2.470E-10	2.96E+05	1.5943E+01	202
15.5 15.5	4932.933	P R 1 2015.51	31463.010	3177.3355	1.022E-01	1.167E-19	1.20E+04	7.5734E-01	203
22.5 22.5	9709.502	Q R 2 2022.51	31403.056	3175.3124	1.009E-00	1.104E-10	6.12E+05	6.5629E-01	204
23.5 22.5	9709.602	Q R 1 2022.51	31400.600	3174.0332	1.473E-02	9.274E-21	3.00E+03	3.7454E-01	205
15.5 16.5	4904.629	P R 1 2016.51	31492.115	3174.4796	4.214E+00	2.41E-10	2.44E+05	3.7200E-01	206
9.5 10.5	2453.149	Q R 1 2010.51	31498.667	3173.0193	1.734E-01	1.007E-19	9.00E+03	2.9033E-01	207
22.5 23.5	9691.321	Q R 2 1023.51	31502.136	3173.4697	1.774E-02	1.11E-20	3.05E+03	4.2172E-01	208
23.5 23.5	9691.321	Q R 1 1023.51	31506.000	3172.9911	1.007E+00	1.10E-10	3.930E+05	4.7357E-01	209
31.5 30.5	16522.271	R R 2 2030.51	31527.110	3170.9550	7.640E-02	4.794E-20	1.05E+05	3.0233E-01	210
13.5 14.5	4371.365	P R 2 2016.51	31540.400	3169.6197	4.527E+00	2.037E-10	3.007E+05	1.4919E-01	211
14.5 14.5	4371.365	P R 1 2016.51	31543.620	3169.2961	2.337E-01	1.46E-10	1.470E+04	7.9156E-01	212
31.5 31.5	16631.946	P R 2 1031.51	31547.443	3168.9120	1.157E-03	7.24E-22	1.50E+03	4.4959E-01	213
32.5 31.5	16631.946	R R 2 1031.51	31553.140	3168.3371	7.156E-02	4.60E-20	9.530E+04	3.1073E-01	214
21.5 21.5	8944.563	Q R 2 2021.51	31564.701	3167.1793	2.410E+00	1.51E-10	6.35E+05	4.39457E-01	215
22.5 21.5	8944.563	Q R 1 2021.51	31569.309	3166.7171	2.035E-02	1.274E-20	3.51E+03	3.0605E-01	216
14.5 15.5	4341.046	P R 1 1015.51	31573.139	3166.3729	4.073E+00	3.054E-10	3.36E+05	1.6275E-01	217
21.5 22.5	8925.622	Q R 2 1022.51	31583.642	3165.2799	2.429E-02	1.52E-10	4.15E+05	4.5746E-01	218
22.5 22.5	8925.622	Q R 1 1022.51	31588.250	3164.8102	2.410E+00	1.51E-10	6.35E+05	4.39457E-01	219
0.5 9.5	2056.550	Q R 1 21 9.51	31595.731	3164.0607	2.137E-01	1.13E-19	1.040E+04	3.1036E-01	220
30.5 37.5	22671.446	S R 2 1037.51	31611.531	3162.4073	2.443E-02	1.53E-23	1.027E+02	1.0166E-01	221
12.5 13.5	3041.676	P R 2 2013.51	31617.404	3161.0990	5.103E-00	3.19E-10	3.17E+05	1.5917E-01	222
13.5 13.5	3041.676	P R 1 2013.51	31620.425	3161.5977	2.974E-01	1.064E-19	1.71E+04	8.3029E-01	223
30.5 29.5	15709.237	R R 2 2029.51	31633.547	3160.2062	1.096E-01	6.467E-20	1.70E+05	2.4240E-01	224
20.5 20.5	8206.027	Q R 2 2020.51	31641.266	3159.5152	3.031E+00	1.90E-10	4.57E+05	4.1002E-01	225
21.5 20.5	8206.027	Q R 1 2020.51	31645.722	3159.0702	2.779E-02	1.74E-10	4.00E+03	3.9002E-01	226
13.5 14.5	3010.759	P R 1 1014.51	31651.343	3158.5052	5.540E+00	3.47E-10	3.17E+05	1.5269E-01	227
30.5 30.5	15600.670	Q R 2 1030.51	31656.113	3158.2320	1.729E-03	1.004E-21	1.037E+03	4.5055E-01	228
31.5 30.5	15600.670	R R 1 1030.51	31659.760	3157.4695	1.033E-01	6.474E-20	1.06E+05	3.0070E-01	229
20.5 21.5	8106.350	Q R 2 1021.51	31660.931	3157.5523	3.291E-02	2.00E-20	4.94E+03	4.4514E-01	230
21.5 21.5	8106.350	Q R 1 1021.51	31665.395	3157.1000	3.059E+00	1.917E-10	4.33E+05	4.3330E-01	231
7.5 0.5	1694.914	Q R 1 21 0.51	31690.020	3154.6534	2.609E-01	3.53E-19	1.35E+04	3.3290E-01	232
11.5 12.5	3344.522	P R 2 2012.51	31691.411	3154.5157	5.645E+00	3.53E-10	3.26E+05	1.2659E-01	233
12.5 12.5	3344.522	P R 1 2012.51	31694.220	3154.2357	3.752E-01	2.35E-19	2.00E+04	8.7420E-01	234
19.5 19.5	7494.040	Q R 2 2019.51	31713.653	3152.3033	3.750E+00	2.35E-10	4.70E+05	3.9302E-01	235
20.5 19.5	7494.040	Q R 1 2019.51	31717.951	3151.0761	3.764E-02	2.35E-20	4.56E+03	4.1304E-01	236
12.5 13.5	3311.902	P R 1 1013.51	31726.769	3151.0801	6.264E+00	3.00E-10	3.20E+05	4.1261E-01	237
29.5 20.5	14705.263	R R 2 2020.51	31733.344	3150.3472	1.541E-01	9.66E-20	1.20E+05	2.0247E-01	238
19.5 20.5	7474.376	Q R 2 1020.51	31736.125	3150.2696	4.422E-02	2.73E-20	9.60E+03	4.5095E-01	239
23.5 20.5	7474.376	Q R 1 1020.51	31739.423	3149.9430	3.015E+00	2.30E-10	4.60E+05	4.1314E-01	240
29.5 29.5	14764.034	P R 2 1029.51	31754.173	3148.2006	2.554E-03	1.60E-21	2.11E+03	4.5097E-01	241
37.5 36.5	21633.010	S R 2 1036.51	31759.597	3147.7429	4.274E-05	2.67E-20	2.394E+02	1.00437E-01	242
30.5 29.5	14764.034	R R 1 1029.51	31759.733	3147.7294	1.470E-01	9.21E-20	1.17E+05	2.9002E-01	243
10.5 11.5	2800.525	P R 2 2011.51	31762.412	3147.4619	6.127E+00	3.04E-10	3.36E+05	1.10217E-01	244
11.5 11.5	2800.525	P R 1 2011.51	31765.021	3147.2054	4.690E-01	2.94E-19	2.35E+04	9.24097E-01	245
6.5 7.5	1368.720	Q R 1 21 7.51	31781.413	3145.5921	3.151E-01	1.97E-19	1.69E+04	3.5779E-01	246
12.5 10.5	6011.055	Q R 2 2010.51	31701.956	3145.5204	4.505E+00	2.074E-10	4.90E+05	3.7362E-01	247

19.5	10.5	6011.055	Q	1	2110.51	31706.009	3145.1192	5.849E-02	3.164E-20	5.217E+03	4.20701E-01	240
11.5	12.5	2064.009	P	1	1112.51	31799.556	3143.7972	6.022E+00	9.274E-10	3.402E+05	1.32510E+01	249
10.5	19.5	6790.493	Q	2	1119.51	31803.310	3143.4150	5.905E-62	3.691E-20	6.370E+03	0.74397E-01	250
19.5	19.5	6790.693	Q	0	1	1119.51	31807.452	4.600E+00	2.930E-19	4.019E+05	3.93012E+01	251
20.5	27.5	13901.320	R	2	2127.51	31826.709	3141.1051	2.143E-01	1.343E-19	1.390E+05	2.72512E+01	252
9.5	10.5	2450.279	P	2	2110.51	31830.303	3140.7425	6.510E+05	0.800E-10	1.340E+05	1.07700E+01	253
10.5	16.5	2450.279	Q	1	2110.51	31832.700	3140.5061	5.016E-61	3.644E-19	2.081E+04	9.00044E-01	254
17.5	17.5	6157.054	Q	2	2117.51	31846.760	3139.1767	5.520E+00	3.400E-10	5.109E+05	3.53391E+01	255
20.5	20.5	13060.205	R	0	2	2120.51	3139.0222	3.339E-03	2.330E-21	2.610E+03	4.66291E-01	256
10.5	17.5	6157.054	R	1	2117.51	31853.222	3138.7061	6.700E-02	4.204E-20	5.071E+03	4.66359E-01	257
29.5	20.5	13060.205	R	1	1120.51	31853.291	3138.4037	2.055E-01	1.200E-19	1.200E+07	2.00050E+01	258
11.5	10.5	6135.500	Q	2	1110.51	31860.613	3136.9747	7.769E-02	4.070E-20	7.250E+03	4.91600E-01	259
10.5	11.5	2413.613	Q	1	1111.51	31869.666	3136.0927	3.367E+00	4.617E-10	3.516E+05	1.22402E+01	260
5.5	6.5	1070.509	Q	1	21	6.51	3136.0672	3.752E-01	2.352E-19	2.102E+04	3.06410E-01	261
10.5	10.5	6135.500	Q	0	1	1110.51	3136.5066	5.569E+00	3.553E-10	5.010E+05	3.72011E+01	262
8.5	9.5	2056.353	P	2	21	9.51	3136.3516	6.764E+00	4.240E-10	3.532E+05	9.72727E+00	263
9.5	9.5	2056.353	Q	1	21	9.51	3136.1373	7.146E-61	4.479E-19	3.359E+04	1.04530E+00	264
36.5	35.5	20600.506	S	2	1135.51	3139.447	3134.0406	7.124E-05	4.465E-23	3.000E+02	1.79406E-01	265
16.5	16.5	5533.620	Q	0	2	2116.51	3133.2356	6.544E+00	4.102E-10	5.379E+05	3.33129E+01	266
27.5	26.5	12990.371	Q	1	2126.51	3132.0639	3132.0639	0.930E-62	5.539E-20	6.051E+03	4.65976E-01	267
16.5	17.5	5510.159	Q	2	1117.51	3130.106	3130.9331	1.013E-01	6.360E-20	0.209E+03	5.11063E-01	269
17.5	17.5	5510.159	Q	0	1	1117.51	3130.5021	6.762E+00	4.230E-10	5.210E+05	3.52594E+01	270
27.5	27.5	12976.943	Q	2	1127.51	3133.009	3130.5021	5.306E-63	3.374E-21	2.759E+03	4.73555E-01	271
9.5	10.5	2015.036	P	1	1110.51	3136.741	3130.4276	7.790E+00	4.806E-10	3.020E+05	1.12265E+01	272
20.5	27.5	12976.943	R	1	1127.51	3136.530	3129.0015	2.036E-01	1.770E-19	1.404E+05	2.70072E+01	273
4.5	5.5	026.013	Q	1	21	5.51	3128.5267	4.309E-01	2.751E-19	2.019E+04	4.10930E-01	274
7.5	8.5	1693.290	Q	2	21	8.51	3128.2936	6.055E+00	4.297E-10	3.811E+05	0.66026E+00	275
0.5	0.5	1693.290	Q	0	1	21	8.51	0.707E-01	5.450E-19	4.077E+04	1.11050E+00	276
15.5	15.5	4930.902	Q	2	2115.51	3128.1015	3127.6939	7.629E+00	4.702E-10	5.549E+05	3.12030E+01	277
16.5	15.5	4930.902	Q	1	2115.51	3127.5416	3127.5416	1.150E-01	7.211E-20	7.077E+03	4.67317E-01	278
15.5	16.5	4915.197	Q	2	1116.51	3125.2703	3125.2703	1.319E-01	0.245E-20	9.500E+03	5.32052E-01	279
16.5	16.5	4915.197	Q	0	1	1116.51	3124.9267	7.943E+00	4.970E-10	5.605E+05	3.32314E+01	280
26.5	25.5	12137.370	R	2	2125.51	3124.5910	3124.5910	3.960E-61	2.405E-19	1.627E+05	2.52636E+01	281
0.5	9.5	1650.790	P	1	11	9.51	3123.9470	0.003E+00	5.064E-10	3.745E+05	1.02100E+01	282
6.5	7.5	1367.617	P	2	21	7.51	3122.5733	6.744E+00	4.227E-10	3.500E+05	7.59906E+00	283
16.5	16.5	4377.619	Q	0	2	2114.51	3122.5733	0.750E+00	5.404E-10	5.713E+05	2.92491E+01	284
26.5	26.5	12115.590	Q	2	1126.51	3122.6677	3122.6669	7.602E-03	4.015E-21	3.334E+03	4.01466E-01	285
7.5	7.5	1367.617	Q	1	21	7.51	3122.4030	1.051E+00	6.590E-19	5.020E+04	1.20092E+00	286
15.5	14.5	4377.619	Q	1	2114.51	31219.125	3122.2007	1.407E-01	9.322E-20	9.105E+03	5.12512E-01	287
27.5	26.5	12115.590	R	1	1126.51	3121.935	3121.9542	3.460E-61	2.420E-19	1.519E+05	2.60092E+01	288
35.5	34.5	15597.902	S	2	1134.51	3120.345	3121.3293	1.136E-64	7.123E-23	3.016E+02	1.70754E-01	289
3.5	4.5	600.194	Q	1	21	4.51	3119.5950	4.996E-61	3.131E-19	3.767E+04	4.32924E-01	290
14.5	15.5	4351.310	Q	2	1115.51	3119.9973	3119.9973	1.609E-01	1.050E-19	1.095E+04	5.57613E-01	291
15.5	15.5	4351.310	Q	0	1	1115.51	3119.6669	9.171E+00	5.740E-10	5.577E+05	3.12011E+01	292
7.5	0.5	1321.252	P	1	11	0.51	3117.0005	0.194E+00	5.136E-10	3.060E+05	9.19255E+00	293
13.5	13.5	3046.059	Q	2	2113.51	3117.7702	3117.7702	9.060E+00	6.104E-10	5.064E+05	2.72100E+01	294
14.5	13.5	3046.059	Q	1	2113.51	3117.4571	3117.4571	1.945E-61	1.319E-19	1.054E+04	5.40150E-01	295
25.5	24.5	11299.250	Q	2	2124.51	3117.2654	3117.2654	5.203E-61	3.317E-19	1.743E+05	2.42675E+01	296
5.5	6.5	1077.054	P	2	21	6.51	3117.0594	6.405E+00	4.019E-10	3.737E+05	6.52103E+00	297
6.5	6.5	1077.054	Q	1	21	6.51	3117.0594	1.255E+00	7.045E-19	6.226E+04	1.29194E+00	298
25.5	25.5	11277.107	P	0	2	1125.51	3115.1141	1.006E-02	6.005E-21	3.556E+03	4.91247E-01	299
13.5	14.5	3019.156	Q	2	1114.51	3115.0709	3115.0709	2.147E-01	1.346E-19	1.267E+04	5.05109E-01	300

Table 9 (Contd.)

J' J''	Lower energy vacuum cm ⁻¹	Transition	Frequency vacuum cm ⁻¹	Wavelength STP angstroms	Intensity cm ⁻² atm ⁻¹	Intensity cm/molecule T = 4600 K	Einstein A sec ⁻¹	Line strength	Number
14.5 14.5	3019.156 -	Q 1 1114.51	32095.029	3114.7633	1.042E+01	6.520E-10	5.739E+05	2.91605E+01	301
26.5 25.5	11277.107 -	R 0 1 1025.51	32097.380	3114.6158	5.170E-01	3.245E-19	1.631E+05	2.50004E+01	302
12.5 12.5	3360.000 -	Q 2 2112.51	32110.200	3113.3722	1.031E+01	6.050E-10	6.002E+05	2.51606E+01	303
2.5 3.5	629.272 -	Q 0 1 21 3.51	32113.213	3113.0001	5.417E-01	3.399E-19	5.175E+04	6.60599E-01	304
13.5 12.5	3160.000 -	Q 0 1 2112.51	32113.222	3113.0792	2.416E-01	1.514E-19	1.232E+04	5.71279E-01	305
6.5 5.5	824.525 -	P 0 2 21 5.51	32122.605	3112.1032	5.032E+00	3.656E-10	3.705E+05	5.43172E+00	306
6.5 7.5	1026.730 -	P 0 1 11 7.51	32123.403	3112.0925	0.095E+00	5.074E-10	3.997E+05	0.17200E+00	307
5.5 5.5	824.525 -	P 0 1 21 5.51	32123.609	3112.0658	1.478E+00	9.261E-19	7.991E+04	1.30079E+00	308
24.5 23.5	10404.962 -	R 0 2 2123.51	32139.570	3110.5270	6.946E-01	4.350E-19	1.052E+05	2.32710E+01	309
12.5 13.5	3319.355 -	Q 0 2 1113.51	32139.725	3110.5120	2.711E-01	1.700E-19	1.470E+04	6.16716E-01	310
13.5 13.5	3319.355 -	Q 0 1 1113.51	32142.747	3110.2196	1.163E+01	7.209E-10	5.000E+05	2.71260E+01	311
36.5 33.5	18602.331 -	S 0 2 1133.51	32149.545	3109.5610	1.706E-04	1.119E-22	4.311E+02	1.70260E-01	312
12.5 11.5	2004.110 -	Q 0 2 2111.51	32151.022	3109.3416	1.106E+01	7.435E-10	6.120E+05	2.31170E+01	313
24.5 24.5	10402.394 -	R 0 2 1124.51	32162.139	3109.0651	3.039E-01	1.905E-19	1.447E+04	6.06410E-01	314
25.5 24.5	10402.394 -	R 0 1 1124.51	32167.150	3107.0591	1.520E-02	9.530E-21	4.744E+05	5.01057E-01	315
3.5 4.5	608.100 -	P 0 2 21 4.51	32173.237	3107.5617	6.046E-01	3.140E-10	3.019E+05	4.33399E+00	316
4.5 4.5	608.100 -	P 0 1 21 4.51	32171.290	3107.6608	7.705E+00	1.069E-10	1.037E+05	1.40361E+00	317
5.5 4.5	707.450 -	P 0 1 11 6.51	32180.756	3106.6459	7.768E+00	4.069E-10	4.141E+05	7.15200E+00	318
11.5 12.5	2032.405 -	Q 0 2 1112.51	32183.440	3106.2046	3.331E-01	2.127E-19	1.737E+04	6.52643E-01	319
1.5 2.5	2007.769 -	Q 0 1 21 2.51	32185.069	3106.0512	5.341E-01	3.340E-19	7.355E+04	4.31554E-01	320
12.5 12.5	2052.405 -	Q 0 1 1112.51	32186.266	3106.0151	1.275E+01	7.992E-10	6.025E+05	2.50015E+01	321
10.5 10.5	2653.149 -	Q 0 2 2110.51	32189.707	3105.6713	1.282E+01	7.900E-10	6.220E+05	2.10604E+01	322
11.5 10.5	2653.149 -	Q 0 1 2110.51	32192.397	3105.4225	3.706E-01	2.373E-19	1.741E+04	6.46105E-01	323
23.5 22.5	9695.394 -	R 0 2 2122.51	32203.691	3104.3526	9.600E-01	5.641E-19	1.961E+05	2.22737E+01	324
2.5 3.5	429.450 -	P 0 2 21 3.51	32213.092	3103.3503	3.900E+00	2.501E-10	3.035E+05	3.23470E+00	325
3.5 3.5	429.450 -	P 0 1 21 3.51	32214.713	3103.2712	1.910E+00	1.197E-10	1.377E+05	1.55030E+00	326
10.5 11.5	2419.001 -	Q 0 2 1111.51	32221.055	3102.3908	4.215E-01	2.642E-19	2.060E+04	6.93759E-01	327
9.5 9.5	2056.560 -	Q 0 2 21 9.51	32226.095	3102.3677	1.311E+01	0.217E-10	6.293E+05	1.09962E+01	328
11.5 11.5	2419.001 -	Q 0 1 1111.51	32226.464	3102.1396	1.378E+01	0.507E-10	6.139E+05	2.30295E+01	329
10.5 9.5	2056.560 -	Q 0 1 21 9.51	32226.492	3102.1369	4.676E-01	2.931E-19	2.041E+04	6.90930E-01	330
23.5 23.5	9672.162 -	P 0 2 1123.51	32226.524	3102.1334	2.107E-02	1.320E-20	4.563E+03	5.13700E-01	331
24.5 23.5	9672.162 -	R 0 1 1123.51	32231.413	3101.6632	0.910E-01	5.505E-19	1.053E+05	2.31050E+01	332
4.5 5.5	543.575 -	P 0 1 11 5.51	32235.903	3101.2312	7.216E+00	4.523E-10	3.319E+05	6.13344E+00	333
1.5 2.5	209.041 -	P 0 2 21 2.51	32252.060	3099.6807	2.702E+03	1.744E-10	3.404E+05	2.14901E+00	334
5.5 1.5	107.491 -	P 0 1 21 1.51	32253.649	3099.5825	4.156E-01	7.405E-19	1.114E+05	3.1012E-01	335
2.5 2.5	209.041 -	P 0 1 21 2.51	32253.647	3099.5453	2.033E+00	1.274E-10	1.075E+05	1.57735E+00	336
0.5 0.5	1694.914 -	Q 0 2 21 0.51	32254.722	3099.4617	1.329E+01	0.329E-10	6.142E+05	1.69230E+01	337
9.5 0.5	1694.914 -	Q 0 1 21 0.51	32256.902	3099.2122	5.723E-01	3.507E-19	2.450E+04	7.41400E-01	338
9.5 10.5	2019.633 -	Q 0 2 1110.51	32261.029	3098.9150	5.191E-01	3.253E-19	2.469E+04	7.41015E-01	339
22.5 21.5	9931.446 -	R 0 2 2121.51	32262.011	3098.7215	1.151E+00	7.213E-22	5.063E+05	2.12757E+01	340
33.5 32.5	17622.044 -	S 0 2 1132.51	32262.292	3098.6955	2.740E-04	1.723E-22	5.063E+05	1.70036E-01	341
10.5 10.5	2019.633 -	Q 0 1 1110.51	32263.426	3098.5056	1.442E+01	9.030E-10	6.236E+05	2.09700E+01	342
7.5 7.5	1360.720 -	Q 0 2 21 7.51	32281.619	3096.0366	1.310E+01	0.209E-10	6.362E+05	1.40431E+01	343
0.5 7.5	1360.720 -	Q 0 1 21 7.51	32281.579	3096.0512	6.920E-01	4.342E-19	2.991E+04	7.97604E-01	344
22.5 22.5	8907.090 -	P 0 2 1122.51	32285.559	3096.4612	2.009E-02	1.011E-20	5.160E+03	5.27171E-01	345
.5 1.5	107.751 -	P 0 2 21 1.51	32286.475	3096.3734	1.470E+00	9.264E-19	3.970E+05	1.10199E+00	346

1.5	1.5	107.751	P	0	1	21	1.51	32206.027	3096.3396	1.906E+00	1.245E-10	2.667E+05	1.050E+00	340
3.5	4.5	355.105	P	1	11	4.51		32209.066	3096.1250	6.44E+00	6.44E-10	4.56E+05	5.121E+00	341
23.5	22.5	9907.090	P	1	1022.51			32298.311	3096.0855	1.145E+00	7.374E-19	1.95E+05	2.28016E+01	350
8.5	9.5	1654.577	P	2	11	9.51		32295.059	3095.5503	6.340E-01	3.379E-19	2.95E+04	7.9554E-01	351
9.5	9.5	1654.577	P	0	1	11	9.51	32297.240	3095.3414	1.403E+01	9.293E-10	6.30E+05	1.09017E+01	352
6.5	6.5	1070.509	P	0	2	21	6.51	32354.695	3094.6269	1.240E+01	9.191E-10	6.33E+05	1.27554E+01	353
7.5	6.5	1070.509	P	0	1	21	6.51	32356.433	3094.4605	0.291E-01	5.194E-19	3.60E+04	0.59222E-01	354
.5	.5	126.449	P	0	1	21	.51	32314.091	3093.7271	1.023E+00	1.442E-10	6.010E+05	1.3333E+00	355
21.5	20.5	0193.990	P	0	2	2020.51		32315.276	3093.6139	1.440E+00	9.167E-19	2.167E+05	2.02760E+01	356
5.5	5.5	024.013	P	0	2	21	5.51	32323.000	3092.7476	1.142E+01	7.155E-10	6.25E+05	1.06647E+01	357
6.5	5.5	024.013	P	0	1	21	5.51	32325.320	3092.6524	9.777E-01	6.324E-19	4.54E+04	9.2370E-01	358
7.5	8.5	1324.291	P	0	2	11	8.51	32326.047	3092.5020	7.709E-01	4.312E-19	3.70E+04	0.50647E-01	359
8.5	8.5	1324.291	P	0	1	11	8.51	32329.007	3092.3953	1.407E+01	9.319E-10	6.34E+05	1.60234E+01	360
4.5	4.5	604.194	P	0	2	21	4.51	32330.736	3091.3693	9.516E+00	6.215E-10	6.095E+05	0.50160E+00	361
21.5	21.5	0169.066	P	0	2	1021.51		32339.390	3091.3060	1.329E-02	2.443E-20	5.04E+03	5.42150E-01	362
5.5	4.5	600.194	P	0	1	21	4.51	32340.020	3091.2466	1.120E+00	7.049E-19	5.77E+04	9.05130E-01	363
2.5	3.5	201.922	P	0	1	11	3.51	32349.505	3091.1943	5.491E+00	3.442E-10	4.95E+05	4.13062E+00	364
22.5	21.5	0169.066	P	0	2	11	21.51	32344.005	3090.9657	1.451E+00	9.092E-19	2.04E+05	2.10763E+01	365
.5	.5	126.291	P	0	2	21	.51	32347.934	3090.4902	1.025E+00	1.344E-10	4.02E+05	1.3333E+00	366
1.5	.5	126.291	P	0	1	21	.51	32340.207	3090.4565	9.105E-01	5.707E-19	1.264E+05	6.6645E-01	367
3.5	3.5	429.275	P	0	2	21	3.51	32349.150	3090.3741	8.030E+00	5.030E-10	5.04E+05	6.52912E+00	368
4.5	3.5	429.275	P	0	1	21	3.51	32350.253	3090.2735	1.250E+00	7.315E-19	7.315E+04	1.02790E+00	369
6.5	7.5	1029.092	P	0	2	11	7.51	32354.112	3089.9001	9.249E-01	5.02E-19	4.65E+04	9.31010E-01	370
1.5	1.5	107.691	P	0	2	21	1.51	32354.610	3089.0717	3.609E+00	2.312E-10	4.94E+05	2.75252E+00	371
2.5	2.5	204.769	P	0	2	21	2.51	32354.907	3089.8544	5.491E+00	7.041E-10	5.40E+05	6.5550E+00	372
2.5	1.5	107.691	P	0	1	21	1.51	32354.907	3089.0156	1.251E+00	7.041E-19	1.124E+05	9.3723E-01	373
3.5	2.5	204.769	P	0	1	21	2.51	32355.050	3089.7770	1.325E+00	0.304E-19	9.221E+04	1.03070E+00	374
7.5	7.5	1029.092	P	0	1	11	7.51	32355.421	3089.7342	1.449E+00	9.007E-10	6.35E+05	1.6734E+01	375
20.5	19.5	7403.075	P	0	2	2010.51		32363.410	3089.0116	1.799E+00	1.127E-10	2.765E+05	1.9277E+01	376
32.5	31.5	16660.617	P	0	2	1031.51		32366.021	3088.6050	4.169E-04	2.813E-22	5.094E+02	1.70065E-01	377
5.5	6.5	769.216	P	0	2	11	6.51	32379.405	3087.3422	1.110E+00	6.950E-19	5.995E+04	1.01636E+00	378
6.5	6.5	769.216	P	0	1	11	6.51	32380.917	3087.3422	1.365E+01	0.553E-10	6.37E+05	1.26352E+01	379
20.5	20.5	7459.105	P	0	2	1020.51		32380.107	3086.6491	5.291E-02	3.310E-20	5.54923E-01	5.54923E-01	380
1.5	2.5	83.719	P	0	1	11	2.51	32390.059	3086.3945	4.416E+00	2.760E-10	5.77E+05	3.14624E+00	381
21.5	20.5	7459.105	P	0	1	1020.51		32392.643	3086.2245	1.000E+00	1.133E-10	2.180E+05	2.00695E+01	382
4.5	5.5	544.009	P	0	2	11	5.51	32402.322	3085.3217	1.316E+00	0.247E-19	7.90E+04	1.11311E+00	383
5.5	5.5	544.009	P	0	1	11	5.51	32403.435	3085.1995	1.233E+01	7.720E-10	6.216E+05	1.05264E+01	384
19.5	10.5	6001.926	P	0	2	2010.51		32406.575	3084.9977	2.201E+00	1.379E-10	2.35E+05	1.02765E+01	385
1.5	.5	126.449	P	0	2	21	.51	32415.452	3084.0520	9.124E-01	5.710E-19	1.212E+05	6.6664E-01	386
3.5	4.5	355.900	P	0	2	11	4.51	32422.526	3083.3900	1.543E+00	9.674E-19	1.102E+05	1.22125E+00	387
4.5	4.5	355.900	P	0	1	11	4.51	32423.579	3083.2794	1.055E+01	6.012E-10	6.023E+05	0.41697E+00	388
19.5	19.5	6776.431	P	0	2	1019.51		32432.070	3082.4726	7.057E-02	4.423E-20	7.50E+03	5.7767E-01	389
20.5	19.5	6776.431	P	0	1	1019.51		32436.360	3082.0641	2.224E+00	1.394E-10	2.254E+05	1.90611E+01	390
.5	1.5	0.000	P	0	1	11	1.51	32440.500	3081.6677	3.360E+00	2.111E-10	0.611E+05	2.35645E+00	391
2.5	3.5	202.370	P	0	2	11	3.51	32440.900	3081.6259	1.702E+00	1.117E-10	1.610E+05	1.31651E+00	392
3.5	3.5	202.370	P	0	1	11	3.51	32441.091	3081.5479	0.369E+00	5.246E-10	5.700E+05	6.31440E+00	393
10.5	17.5	6140.942	P	0	2	2017.51		32444.064	3081.2565	2.652E+00	1.642E-10	2.443E+05	1.47274E+01	394
2.5	1.5	107.751	P	0	2	21	1.51	32455.599	3080.2370	1.092E+00	1.194E-10	1.711E+05	1.41290E+00	395
1.5	2.5	83.920	P	0	2	11	2.51	32457.901	3080.0117	2.016E+00	1.262E-10	2.646E+05	1.45015E+00	396
2.5	2.5	83.920	P	0	1	11	2.51	32450.560	3079.9501	5.000E+00	3.903E-10	5.53E+05	4.25110E+00	397
31.5	26.5	15716.026	P	0	2	1030.51		32463.363	3079.5011	6.227E-04	3.903E-22	6.37E+02	1.79360E-01	398
10.5	10.5	6122.620	P	0	2	1010.51		32471.003	3070.7594	9.311E-02	5.016E-20	8.51E+03	5.90646E-01	399
.5	1.5	.056	P	0	2	11	1.51	32474.170	3070.4762	2.230E+00	1.403E-10	5.735E+05	1.56667E+00	400

Table 9 (Contd).

J' J''	Lower energy vacuum cm ⁻¹	Transition	Frequency vacuum cm ⁻¹	Wavelength STP angstroms	Intensity cm ⁻² atm ⁻¹	Intensity cm/molecule	Einstein sec ⁻¹	A Line strength	Number
1.5 1.5	.056 +	Q 1 1 1.5	32474.523	3070.4920	3.207E+00	2.010E-10	6.100E+05	2.24021E+00	401
19.5 10.5	6122.620 +	R 1 1 10.5	32475.317	3070.3675	3.694E+00	1.600E-10	5.346E+05	1.00500E+01	402
17.5 16.5	5525.697 -	R 2 2 16.5	32476.417	3070.6737	3.146E+00	1.972E-10	2.523E+05	1.62723E+01	403
3.5 2.5	209.061 -	R 2 2 2.5	32409.304	3077.0346	2.933E+00	1.030E-10	2.050E+05	2.27273E+00	404
17.5 17.5	5490.452 -	R 2 2 17.5	32505.661	3075.4937	1.219E-01	7.640E-20	9.707E+03	6.22121E-01	405
16.5 15.5	4932.933 +	R 2 2 15.5	32507.330	3075.3350	3.669E+00	2.300E-10	2.592E+05	1.52006E+01	406
10.5 17.5	5690.452 -	R 1 1 17.5	32509.624	3075.1100	3.212E+00	2.013E-10	2.424E+05	1.70304E+01	407
6.5 3.5	429.450 -	R 2 2 3.5	32517.473	3074.3765	3.936E+00	2.467E-10	2.313E+05	3.20633E+00	408
15.5 16.5	4371.365 -	R 2 2 16.5	32531.710	3073.0310	4.214E+00	2.641E-10	2.650E+05	1.45537E+01	409
16.5 16.5	4904.629 +	R 2 2 16.5	32535.634	3072.6483	1.501E-01	9.912E-20	1.109E+04	6.40424E-01	410
17.5 16.5	4904.629 +	R 1 1 16.5	32539.420	3072.3020	3.770E+00	2.363E-10	2.490E+05	1.60326E+01	411
5.5 4.5	600.100 -	R 2 2 4.5	32540.433	3072.2072	4.017E+00	3.019E-10	2.690E+05	4.10373E+00	412
1.5 1.5	0.000 -	R 2 2 1.5	32541.941	3072.0806	1.982E+00	0.707E-19	1.003E+05	9.0002E-01	413
2.5 1.5	0.000 -	R 1 1 1.5	32542.404	3072.0131	9.434E-01	5.913E-19	0.091E+04	6.62669E-01	414
14.5 13.5	3041.676 +	R 2 2 13.5	32551.652	3071.1403	4.751E+00	2.970E-10	2.711E+05	1.32577E+01	415
16.5 20.5	14790.667 +	S 2 2 20.5	32552.137	3071.1025	9.197E-04	5.764E-22	7.063E+02	1.70594E-01	416
6.5 5.5	024.525 +	R 2 2 5.5	32550.679	3070.4955	5.521E+00	3.400E-10	2.629E+05	5.17021E+00	417
2.5 2.5	03.719 +	R 2 2 2.5	32559.631	3070.3956	1.766E+00	1.107E-10	1.557E+05	1.27205E+00	418
3.5 2.5	03.719 +	R 1 1 2.5	32560.452	3070.3102	2.124E+00	1.312E-10	1.404E+05	1.5400E+00	419
15.5 15.5	4341.046 -	R 2 2 15.5	32561.229	3070.2450	2.031E-01	1.273E-19	1.271E+04	6.77930E-01	420
16.5 15.5	4341.046 -	R 1 1 15.5	32564.051	3069.9053	4.346E+00	2.724E-10	2.561E+05	1.50062E+01	421
13.5 12.5	3344.522 -	R 2 2 12.5	32567.242	3069.6700	5.261E+00	3.297E-10	2.756E+05	1.22503E+01	422
7.5 6.5	1077.054 -	R 2 2 6.5	32572.405	3069.1040	6.014E+00	7.772E-10	2.737E+05	6.10407E+00	423
3.5 3.5	201.922 -	R 2 2 3.5	32576.504	3068.0053	1.709E+00	1.129E-10	1.220E+05	1.34301E+00	424
4.5 3.5	201.922 -	R 1 1 3.5	32577.557	3068.7061	3.334E+00	2.090E-10	1.031E+05	2.52505E+00	425
12.5 11.5	2000.525 +	R 2 2 11.5	32570.555	3068.6120	5.714E+00	3.505E-10	2.791E+05	1.12616E+01	426
8.5 7.5	1367.617 +	R 2 2 7.5	32582.019	3068.2959	6.310E+00	3.955E-10	2.773E+05	7.11004E+00	427
14.5 14.5	3010.759 +	R 2 2 14.5	32582.570	3068.2339	2.505E-01	1.620E-19	1.464E+04	7.11106E-01	428
11.5 10.5	2950.279 -	R 2 2 10.5	32585.653	3067.9436	6.074E+00	3.007E-10	2.610E+05	1.02315E+01	429
15.5 10.5	3010.759 +	R 1 1 10.5	32585.905	3067.9124	6.932E+00	3.091E-10	2.619E+05	1.39060E+01	430
9.5 8.5	1893.290 -	R 2 2 8.5	32587.372	3067.7010	6.404E+00	4.014E-10	2.006E+05	0.20015E+00	431
10.5 9.5	2054.353 +	R 2 2 9.5	32580.503	3067.6670	6.315E+00	3.950E-10	2.016E+05	9.22020E+00	432
6.5 4.5	395.105 +	R 2 2 4.5	32591.026	3067.3626	1.660E+00	1.046E-10	9.577E+04	1.21733E+00	433
5.5 4.5	355.105 +	R 1 1 4.5	32593.109	3067.2510	4.445E+00	2.707E-05	2.337E+05	3.55940E+00	434
13.5 13.5	3311.902 -	R 2 2 13.5	32599.703	3066.6110	3.262E-01	2.044E-19	1.695E+04	7.40441E-01	435
14.5 13.5	3311.902 -	R 1 1 13.5	32603.003	3066.3109	5.491E+00	3.441E-10	2.664E+05	1.29024E+01	436
5.5 5.5	543.575 -	R 2 2 5.5	32605.006	3066.1100	1.475E+00	9.240E-19	7.527E+04	1.25109E+00	437
6.5 5.5	543.575 -	R 1 1 5.5	32606.557	3065.9766	5.370E+00	3.374E-10	2.352E+05	4.61326E+00	438
12.5 12.5	2466.009 +	R 2 2 12.5	32612.991	3065.3710	4.000E-01	2.557E-19	1.975E+04	7.90527E-01	439

ignored, our line strengths are identical to those calculated using Earls' formulas. Ignoring these effects does not significantly alter the line strengths for main branch transitions but does lead to large errors at high J for the weaker satellite branch line strengths. Earls' formulas (which ignore centrifugal and higher distortion and Σ - Π interactions) predict consistently smaller line strengths than those calculated by us (which include centrifugal and higher distortion and Σ - Π interactions). In the $^2R_{12}$ branch, Earls' line strengths range from 93% of our line strength at $J'' = 20.5$ to 69% of our line strength at $J'' = 40.5$; in the $^5R_{21}$ branch they range from 78% of our line strength at $J'' = 20.5$ to 46% of our line strength at $J'' = 39.5$. Earls' formulas show intermediate error in this range for the other satellite branches.

Bennett's¹³ line-strength formulas, which include P^4 centrifugal distortion, may be expected to give much more accurate results. Based on our check of Earls' formulas, the line strengths for the $^5R_{21}$ branch should have the largest deviation. Bennett's formula predicts line strengths for this branch which are 1% higher than ours at $J = 1.5$ and decrease to 6% lower at $J = 25.5$; they increase to 2% higher at $J = 39.5$. Examination of the eigenvectors shows that the P^4 term and, to a lesser extent, the $^2\Sigma$ - $^2\Pi$ mixing can contribute an effect of a few percent to the satellite bands line strengths. Thus, the dominant effect in the deviations from Earls' formulas is due to the centrifugal distortion, which is relatively large in a light molecule such as OH.

The conclusion to be drawn from these comparisons is that both the algebraic formulas or our method give accurate main branch line strengths at all experimentally observed J values. Earls' formulas lead to significant errors at high J in the satellite bands. Bennett's formulas give acceptable satellite branch line strengths for most work. However, when the highest accuracy is required, the line strengths from Table 9 should be used.

When our Einstein A coefficients are normalized to the same relative value as those of Chidsey and Crosley,³ the two sets of values differ by at most ± 2 in the last decimal place. As with line strengths, these differences become important only at high J in the satellite branches where many of the relative Einstein A coefficients are quoted to only one significant digit by Chidsey and Crosley. An additional advantage of our Einstein A coefficients in Tables 8 and 9 for quantitative spectroscopy is that they are absolute rather than relative values.

Although we have chosen to present OH line parameters for temperatures of 240 and 4600°K, our computer program can generate $A^2\Sigma$ - $X^2\Pi(0,0)$ band line parameters for any temperature. Table 10 may be used with Tables 8 or 9 and Eqs. (3) and (5) to convert line intensities from these temperatures to any temperature in the 200–6000°K range. Intensities so determined should have the same accuracy as those in Tables 8 and 9. Band intensities at temperatures other than 240 and 4600°K may be calculated by summing the individual line intensities at the desired temperature. Simpler approximate procedures which directly convert from a band intensity at one temperature to a band intensity at another temperature such as Eq. (7-126) in Penner,⁶ give errors of approx. 15% when band intensities at 240 and 4600°K are compared.

Table 10. Rotational partition function Q_R vs temperature T .

T (K)	Q_R	T (K)	Q_R
200	26.71	2000	298.23
240	32.24	2500	373.27
296	40.17	3000	454.19
300	40.75	3500	533.18
500	70.00	4000	612.85
750	107.35	4500	693.14
1000	145.09	4600	709.26
1250	183.08	5000	773.98
1500	221.28	5500	855.28
1750	259.67	6000	936.88

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4. REFERENCES

1. G. H. Dieke and H. M. Crosswhite, *JQSRT* 2, 97 (1962).
2. J. L. Destombes, C. Marliere, and F. Rohart, *J. Molec. Spectrosc.* 67, 93 (1977).
3. I. L. Chidsey and D. R. Crosley, *JQSRT* 23, 187 (1980).
4. J. T. Hougen, *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules*, NBS Monograph 115, U.S. Government Printing Office, Washington, D.C. (1970).
5. J. L. Destombes and C. Marliere-Demuyck, Private communication (1980).
6. S. S. Penner, *Quantitative Molecular Spectroscopy and Gas Emissivities*, Addison-Wesley, Reading, Mass. (1959).
7. K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure IV, Constants of Diatomic Molecules*, Van Nostrand Reinhold, New York (1979).
8. L. T. Earls, *Phys. Rev.* 48, 423 (1935).
9. I. L. Chidsey and D. R. Crosley, "Tables of Calculated Transition Probabilities for the A-X System of OH", Ballistic Research Laboratory Scientific Rep., to be published (1980).
10. K. R. Gorman, *J. Chem. Phys.* 62, 2584 (1974).
11. E. E. Whiting and R. W. Nicholls, *Astrophys. J. Suppl. Series* 27, 1 (1974).
12. I. Kovacs, *Rotational Structure of Diatomic Molecules*, p. 130, Elsevier, New York (1969).
13. R. J. M. Bennett, *Mon. Not. R. Astr. Soc.* 167, 35 (1970).

ERRATUM

The following corrections should be made to Goldman and Gillis¹.

In Eq. (3) and (7) the expression $(2J'+1)$ should be $4(2J'+1)$.
Consequently, all intensities in $\text{cm}^{-1}/\text{atm-cm}$ and $\text{cm}/\text{molecule}$ in Ref. 1
should be multiplied by 4. All other line parameters remain unchanged.

1. A. Goldman and J. R. Gillis, JQSRT 25, 111 (1981).